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The Control of Gold Nanoparticles on Polyester Fibers by Raman Spectrograms in Conditions of Information Uncertainty with Detection Accuracy

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Results of modeling of the Raman spectrograms of polyester fibers are presented when drawing nanoparticles of gold on them. As a result of the carried-out modeling were allocated: initial ranges, background components and the Raman ranges without background components. For simplification of procedures of mathematical modeling it was chosen 7 informative resonant peaks of the received spectrograms. Further processing was carried out only on coordinates of resonant peaks. For detection of reliability of control of nanoparticles of gold on making components of the Raman ranges when using conditions of information uncertainty in work the method of an assessment of multidimensional reliability on joint probability of crossing of dispersions of normal distributions of intensivnost of the Raman spectrograms without nanoparticles and with nanoparticles on fibers depending on wave numbers on all range of their changes is offered. Values of reliability of control on making components of the Raman spectrograms were as a result received and the most exact method for monitoring procedure of nanoparticles of gold on a surface of fibers is revealed.

Keywords: Polyester fiber, Gold nanoparticles, The Raman ranges, Information uncertainty, Mathematical modeling, Background luminescent components, Reliability of control, Probability of crossing of dispersions of normal distributions.

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1. INTRODUCTION

To provide biomedical, therapeutic and protective properties of textile materials using gold nanoparticles arises the need to use the convergence of nano-, bio-, info-, cognitive science, and technology.

In physical effect used Raman light scattering (SERS) [1-2], which is based on plasmon enhancement signal components from the Raman spectrum in the presence of gold nanoparticles. In addition, the applied polarizing effect of the laser beam Raman spectrometer PE fibers with gold nanoparticles, which provides an additional enhancement of the Raman and background fluorescent components of the Raman spectrogram.

2. DESCRIPTION OF THE SUBJECT AND METHODS OF RESEARCH

2.1 Experimental Procedure

To improve the reliability of the control of presence of small amounts of colloidal gold nanoparticles on polyester (PE) fibers used Raman spectrometer, followed by separation of the spectral components of informative and processing on mathematical models in conditions of information uncertainty.

In the experiment, selected PE fiber, which were deposited on gold nanoparticles from a colloidal solution of gold nanoparticles (TU 9154-001-93099853-06 NGOs Biotest). Polyester fiber was selected because of the small amount of the main components of the Raman spectrum. Obtained following fiber samples: samples 0, 1, 2 – without nanoparticles , samples 10, 11 and 12 – to a nanoparticle. Sample 0 - without nanoparticles, sample 1 – without nanoparticles in measuring the polarization of the laser beam, sample 2 – without nanoparticles when measured spectrograms on a single fiber. Sample 10- to 5-nm gold nanoparticles dried in the drying oven, the sample 11- to 10-nm gold nanoparticles dried in natural conditions, the sample was 12- to 10-nm gold nanoparticles dried in a drying oven. The measurements were made with a scanning probe microscope (SPM) with a confocal Raman and fluorescence spectrometer OmegaScope ™.

2.2 The processing of the experimental data

In the first step of the simulation was performed mathematical modeling background components for minimum data spectrograms of the Raman spectrum in the program Mathcad. For example, in Fig. 1 the simulation results for PE fibers with gold nanoparticles [3-5].

Carry out the digitization of all spectrograms by peaks and separately on the background fluorescent constituent fibers in the spectrograms of the program Mathcad and present this data in the form of a matrix.

In matrices W0, W1, W2, and W10, W11, W12 are the coordinates data spectrogram peaks initial starting with the background components of samples 0, 1, 2 fibers without gold nanoparticles samples and PE fibers with 10, 11, 12 gold nanoparticles (Fig. 1a – E10). The first column shows the number of wave peaks, and the second column shows the intensity of the peaks with the back-end components for the initial source spectrograms. Total 7 selected informative peaks on each spectrogram. In matrix S0, S1, S2, and S10, S11, S12 are the coordinates data only peaks without background components of Samples 1, 2, 3 without the fibers and gold nanoparticle samples 10, 11, 12 PE fibers with gold nanoparticles (Fig. 1b). The first column shows the number of wave peaks, and the second column shows the intensity of the peaks without background components spectrograms. In matrix V0, V1, V2 and V10,

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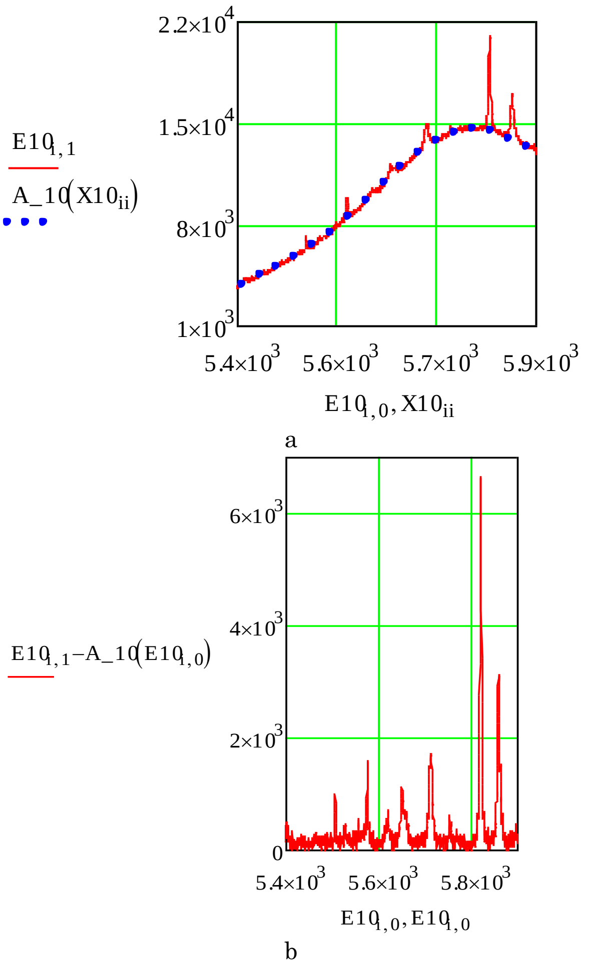

Fig. 1 – Spectrograms Raman Raman scattering in the sample MathCad 10 PE fiber with gold nanoparticles: a – initial spectrum (E10) and simulated background component (A_10 (X10)); b – spectrum without background fluorescent components

V11, V12 are spectrograms background fluorescent component samples 1, 2, 3 without the fibers and gold nanoparticle samples 10, 11, 12 PE fibers with gold nanoparticles (Fig. 1a – A_10 (X10)).

The first column shows the wave numbers that indicate the location of spectrogram peaks $E_{i,0}$. The second column shows the intensity of the background components under the peaks of spectrograms which were obtained by subtracting the intensity of the peaks without background components S of the peak intensities in conjunction with the background components of W by the formulas:

$$V0_{i,1} = W0_{i.1} - S0_{i,1};$$
$$V1_{i,1} = W1_{i.1} - S1_{i,1}; \qquad (1)$$
$$V2_{i,1} = W2_{i.1} - S2_{i,1}.$$

$$V10_{i,1} = W10_{i.1} - S10_{i,1};$$
$$V11_{i,1} = W11_{i.1} - S11_{i,1}; \qquad (2)$$
$$V12_{i,1} = W12_{i.1} - S12_{i,1}.$$

Fig. 2 shows an example matrix for fiber samples 0 and 1. Fig. 3 shows the image data when combined spectrogram peaks. Fig. 4 shows an example matrix for fiber samples 10 and 11.

$$W0 := \begin{pmatrix} 5401.9 & 2359.1 \\ 5505.8 & 2558.2 \\ 5575.4 & 2855.0 \\ 5650 & 2903.9 \\ 5712.5 & 3519.8 \\ 5820.8 & 5851.4 \\ 5859.6 & 4569.3 \end{pmatrix} \quad W1 := \begin{pmatrix} 5400.0 & 3131.1 \\ 5505.3 & 3260.7 \\ 5574.5 & 3389.7 \\ 5649.6 & 3320.1 \\ 5712.1 & 4393.9 \\ 5819.9 & 8402.1 \\ 5857.8 & 5714.8 \end{pmatrix}$$

a

$$S0 := \begin{pmatrix} 5401.9 & 318.6 \\ 5505.8 & 434.9 \\ 5575.4 & 689.4 \\ 5650 & 450.8 \\ 5712.5 & 771.5 \\ 5820.8 & 2685.8 \\ 5859.6 & 1410.0 \end{pmatrix} \quad S1 := \begin{pmatrix} 5400.0 & 508.4 \\ 5505.3 & 749.1 \\ 5574.5 & 959.4 \\ 5649.6 & 674.5 \\ 5712.1 & 1267.4 \\ 5819.9 & 4951.8 \\ 5857.8 & 2340.7 \end{pmatrix}$$

b

$$V0 = \begin{pmatrix} 5401.9 & 2040.5 \\ 5505.8 & 2123.3 \\ 5575.4 & 2165.6 \\ 5650 & 2453.1 \\ 5712.5 & 2748.3 \\ 5820.8 & 3165.6 \\ 5859.6 & 3159.3 \end{pmatrix} \quad V1 = \begin{pmatrix} 5400 & 2622.7 \\ 5505.3 & 2511.6 \\ 5574.5 & 2430.3 \\ 5649.6 & 2645.6 \\ 5712.1 & 3126.5 \\ 5819.9 & 3450.3 \\ 5857.8 & 3374.1 \end{pmatrix}$$

c

Fig. 2 – Coordinates spectrogram peaks fibers without gold nanoparticles: a – the original; b – without background components; c – background components

Fig. 5 shows the image data when combined spectrogram peaks.

In the next stage in the program MathCAD were obtained values of the expectations of the intensities of each peak source spectrograms fibers without nanoparticles YYWi, YYSi, YYVi and of nanoparticles YYYWi, YYYSi, YYYVi, as well as the estimated standard devi ation of the intensity of each peak spectrograms fibers without nanoparticles $\sigma\Delta012W_i$, $\sigma\Delta012S_i$, $\sigma\Delta012V_i$ and gold nanoparticles $\sigma\Delta101112W_i$, $\sigma\Delta101112S_i$ $\sigma\Delta101112V_i$.

3. DESCRIPTION AND ANALYSIS OF RESULTS

Assess the robustness of the control of presence of nanoparticles has been invited to conduct in probability distributions of the intensity of contact with the spectrograms of information uncertainty (uzzy logic) when deciding on the presence of nanoparticles. Distribution parameter of the peak intensities for example, peak 7 i = 6) fiber spectrograms as the nanoparticles and without nanoparticles are shown in Fig. 6.

Here it is seen that the expectations of the intensities of the spectrograms of PE fibers by peaks with i = 0...6 under the influence of gold nanoparticles (line 1) exceeds line 7 of the expectations of the peaks of the spectrograms of PE fibers without nanoparticles in the whole range of changes i = 0...6. For background components with gold nanoparticles Fig. 6a line expecta-

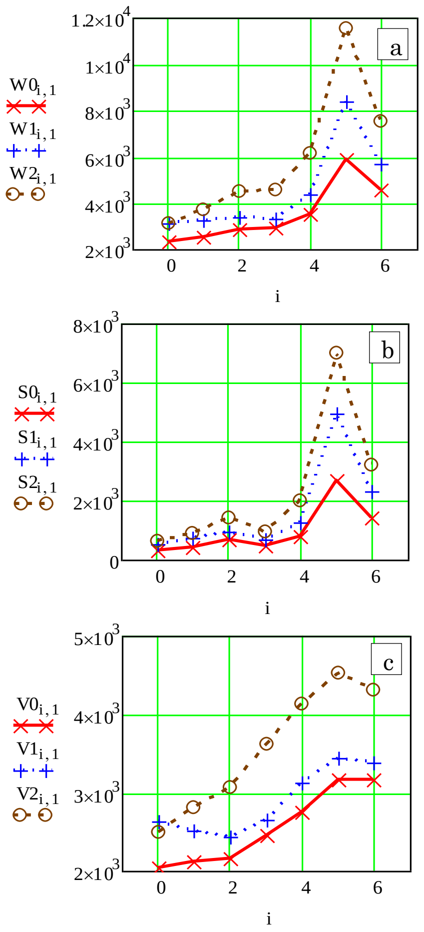

Fig. 3 – Combining spectrogram peaks without gold nanoparticles: a – source; b – without background components; c – background components.

$$W10:=\begin{pmatrix} 5400.9 & 4374.1\\ 5505.3 & 7156.5\\ 5574.9 & 9869\\ 5649.6 & 12165\\ 5712.5 & 14987\\ 5820.4 & 21051\\ 5858.3 & 16985 \end{pmatrix} \qquad W11:=\begin{pmatrix} 5401.4 & 4804.2\\ 5505.8 & 7936.2\\ 5575.4 & 10627\\ 5649.1 & 13380\\ 5713.4 & 17383\\ 5820.4 & 25177\\ 5858.7 & 20668 \end{pmatrix}$$

a

$$S10:=\begin{pmatrix} 5400.9 & 540.6\\ 5505.3 & 1045.5\\ 5574.9 & 1643.0\\ 5649.6 & 1162.0\\ 5712.5 & 1772.7\\ 5820.4 & 6696.7\\ 5858.3 & 3172.5 \end{pmatrix} \qquad S11:=\begin{pmatrix} 5400.0 & 546.5\\ 5505.3 & 1152.3\\ 5575.4 & 1457.1\\ 5649.1 & 1158.1\\ 5713.4 & 2243.5\\ 5820.4 & 7580.3\\ 5858.7 & 3454.8 \end{pmatrix}$$

b

$$V10=\begin{pmatrix} 5400.9 & 3833.5\\ 5505.3 & 6111\\ 5574.9 & 8226\\ 5649.6 & 11003\\ 5712.5 & 13214.3\\ 5820.4 & 14354.3\\ 5858.3 & 13812.5 \end{pmatrix} \qquad V11=\begin{pmatrix} 5400 & 4257.7\\ 5505.3 & 6783.9\\ 5575.4 & 9169.9\\ 5649.1 & 12221.9\\ 5713.4 & 15139.5\\ 5820.4 & 17596.7\\ 5858.7 & 17213.2 \end{pmatrix}$$

c

Fig. 4 – The coordinates of the peaks of the spectrograms of fibers c gold nanoparticles: a – source; b – without background components; c – background components.

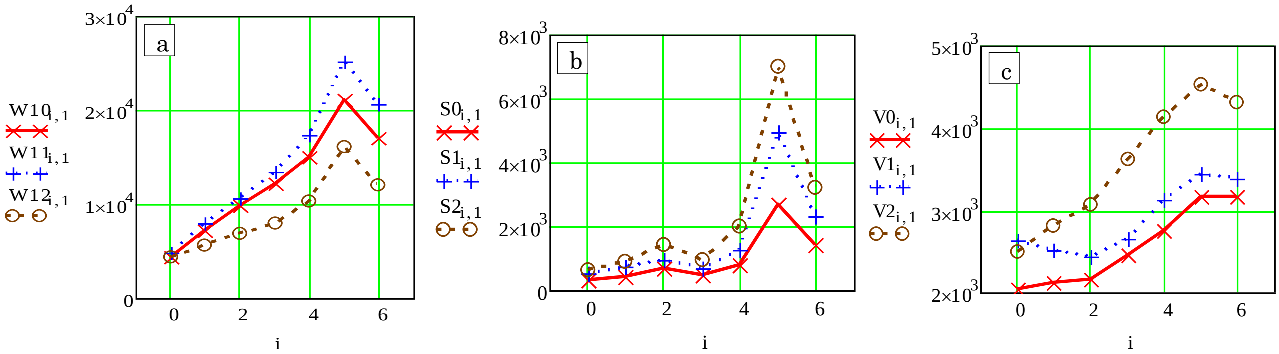

Fig. 5 – Combining spectrogram peaks to gold nanoparticles: a – the original; b – without background components; c – background components

tions clearly exceeds 1 line 7 of expectations without gold nanoparticles. In the original spectrograms with the peaks and background components (Fig. 6b) expectations in line 1 is also significantly higher than expectations in line 7 spectrograms without gold nanoparticles. If we consider only the spectrogram peaks without background components (Fig. 6c), the expectations on line 1 are slightly different from the expectations line 7 without gold nanoparticles.

Also, do not cross the line 3 the minimum values of the peak intensities with $i = 0…6$ background components with gold nanoparticles: a – $V12_{i,1}$ and the original b – $W12_{i,1}$ to 6 lines maximum values of peak intensities with $i = 0…6$ background components without gold nanoparticles: a – $V2_{i,1}$ and the original b – $W2_{i,1}$.

Evaluation of reliability of the multidimensional control of gold nanoparticles on the surface of PE fiber to carry out certain points of intersection of the line modeled variations in the peak intensities of 4 at the line of contact with the minimum spread of the distribution of intensities of 5 for each peak.

Fig. 6 shows the following lines: 1 – line expectations of the peak intensities with $i = 0…6$ with gold

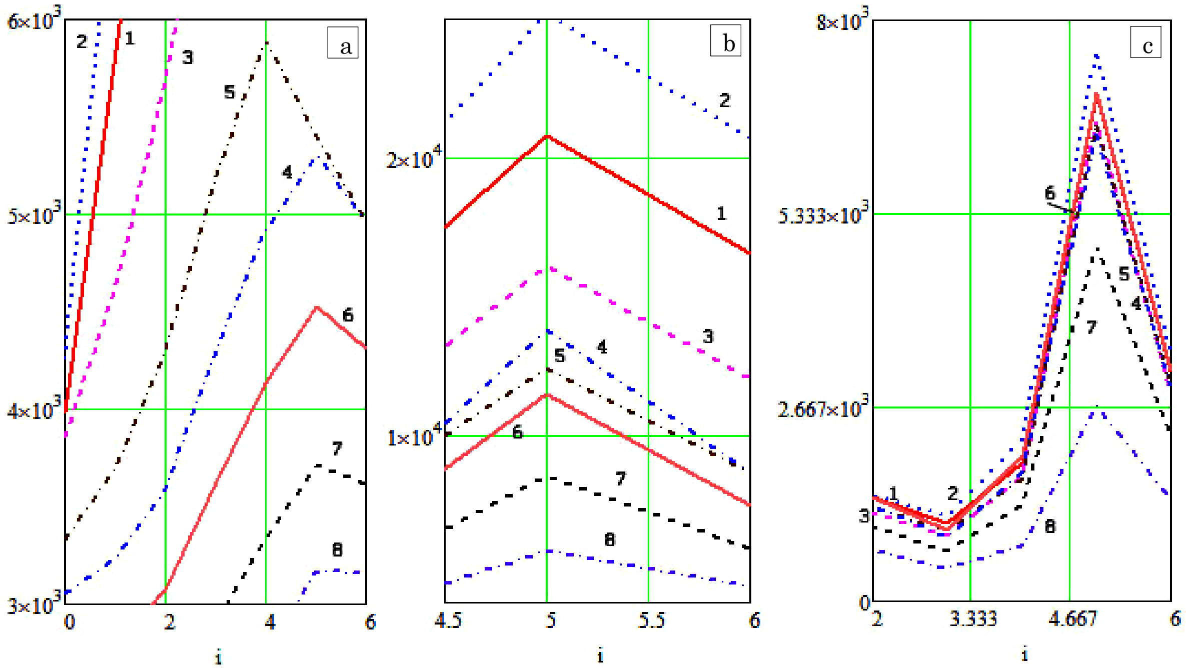

Fig. 6 – Graphs of the intensity parameters of spectrogram peaks for the peak with i = 6a – parameters of peaks spectrograms background components; b – the parameters of the original spectrogram peaks; c – the parameters of spectrogram peaks without background components

nanoparticles: a –$YYYV_i$, b –$YYYW_i$, c –$YYYS_i$; 2 – line the maximum values of the peak intensities with i = 0...6 gold nanoparticles: a – $V11_{i,1}$, b – $W11_{i,1}$ c – $S11_{i,1}$, 3 – line the minimum values of the peak intensities with i = 0...6 with gold nanoparticles: a – $V12_{i,1}$, b – $W12_{i,1}$ c – $S12_{i,1}$, 4 – simulated line variations in the intensity distribution of the peaks with i: = 0...6: a –$YYV_i + y_i.\ \sigma\Delta012Vi$; b – $YYW_i + y_i.\ \sigma\Delta012Wi$; c – $YYS_i + y_i.\ \sigma\Delta012S_i$; 5 – simulated line minimum spread of the distribution of the peak intensities with i: = 0...6: a – $YYYV_i$-$y_i.\ \sigma\Delta101112V_i$; b – $YYYW_i$- $y_i.\ \sigma\Delta101112W_i$; c – $YYYSi$-$y_i.\ \sigma\Delta101112S_i$; 6 – the line of the maximum values of the peak intensities with i: = 0...6 without gold nanoparticles: a – $V2_{i,1}$; b – $W2_{i,1}$; c – $S2_{i,1}$, 7 – the line of the expectations of the peak intensities with i: = 0...6 without gold nanoparticles: a –YYV_i; b –YYW_i; c –YYS_i; 8 – line of minimum intensity values peaks i: = 0...6 without gold nanoparticles: a – $V0_{i,1}$; b – $W0_{i,1}$; c – $S0_{i,1}$; y_i – normal variations in the coefficient of the intensity distribution.

To determine the coefficient yi, used in calculating the point of intersection of lines 4 and 5, we proposed a method that is implemented in the system MathCAD:

$$
\begin{aligned}
y_{W1i} &:= (YYYW_i - YYW_i) / (\sigma\Delta101112W_i + \sigma\Delta012W_i) \\
y_{S1i} &:= (YYYS_i - YYS_i) / (\sigma\Delta101112S_i + \sigma\Delta012S_i) \\
y_{V1i} &:= (YYYV_i - YYV_i) / (\sigma\Delta101112V_i + \sigma\Delta012V_i)
\end{aligned}
\qquad (3)
$$

Evaluation of reliability in the MathCAD held in the following expressions:

$$
\begin{aligned}
&p1W_i = 1 - \mathrm{pnorm}(YYYW_i - y_i \cdot \sigma\Delta101112W_i\ , YYYW_i\ , \sigma\Delta101112W_i), \\
&p2W_i = \mathrm{pnorm}(YYW + y_i \cdot \sigma\Delta012W_i\ , YYW_i\ , \sigma\Delta012W_i\ ). \\
&p1S_i = 1 - \mathrm{pnorm}(YYYS_i - y_i \cdot \sigma\Delta101112S_i\ , YYYS_i\ , \sigma\Delta101112S_i), \\
&p2S_i = \mathrm{pnorm}(YYS + y_i \cdot \sigma\Delta012S_i\ , YYS_i\ , \sigma\Delta012S_i\ ). \\
&p1V_i = 1 - \mathrm{pnorm}(YYYV_i - y_i \cdot \sigma\Delta101112V_i\ , YYYV_i\ , \sigma\Delta101112V_i), \\
&p2V_i = \mathrm{pnorm}(YYV + y_i \cdot \sigma\Delta012V_i\ , YYV_i\ , \sigma\Delta012V_i\ ).
\end{aligned}
\qquad (4)
$$

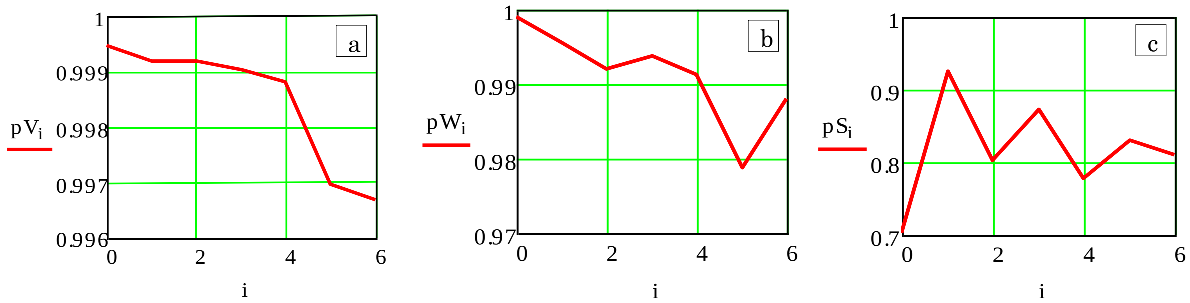

Fig. 7 – The accuracy of the control of the presence of gold nanoparticles: a – on the back-end components of the spectrograms, b – from the peaks to the background components of the spectrograms, c – from the peaks without background components spectrograms

Expression (3-4) were obtained values yi, p1i, p2i for all components of the Raman spectrogram. Results of testing reliability of gold nanoparticles on PE fiber according to (4) shown in Fig. 7.

Data validity checking the presence of gold nanoparticles on the back-end components are shown in Fig. 7a. The range of values of reliability varies from 0.9995 to peak with i = 0 to 0.9967 for the peak with i = 6. These values indicate a very high accuracy of the control of the presence of gold nanoparticles in the PE fibers. Evaluation of the accuracy control of the presence of gold nanoparticles on the original spectrograms with the peaks and background components is shown in Fig. 7b. The range of values of reliability varies from 0.9989 to peak with i = 0 to 0.9790 for the peak with i = 5. These values indicate a very high accuracy of the control of the presence of gold nanoparticles. Monito-ring the availability of gold nanoparticles only on the peaks of the spectrograms without background components gives the lowest reliability and values are shown in Fig. 7c. The range of values of reliability varies from 0.6915 to peak with i = 0 to 0.9262 for the peak with i = 1.

These values indicate a very low reliability of the control of the presence of nanoparticles. Values were determined reliability of the control of generalized parameter values common to i = 0...6 distributions, which the background is at spectrograms and only starting from the peaks have the following meanings: $P\xi v = 0.991546$, $P\xi w = 0.971375$, $P\xi s = 0.720666$.

From these pooled data shows that the highest accuracy of the method has a control for background components, the accuracy and the lowest was obtained in the control on the spectrogram peaks without background components. Thus, as a method of control of gold nanoparticles can be recommended to the definition of a multidimensional credibility in the background components.

4. CONCLUSIONS

1. Due to the large scatter in the values of information parameters in the control of gold nanoparticles on polyester fibers and considerable uncertainty in the laws of their manifestation is the most suitable method for assessing the reliability of monitoring the presence of nanoparticles in probability distributions of the intensity of contact with the spectrograms of information uncertainty (fuzzy logic) when deciding on a nanoparticles.

2. We expand the spectrogram to background fluorescent components and resonance Raman peak intensities of radiation with subsequent mathematical processing to identify the parameters of the normal distribution.

3. To simplify the procedures of mathematical modeling of the data background components, raw spectrogram peaks and intensities of treatment carried out only on the coordinates of the resonance peaks of the spectrograms. Joined 7 informative resonance peaks.

4. To eliminate uncertainty and identify patterns in the distribution of the parameters of the spectrograms assessed values of the distribution parameters of the peak intensities as a function of the spectrograms of wave numbers (frequencies) as the background components and raw spectrograms and peak intensities for fibers without nanoparticles and nanoparticles.

5. Evaluated multidimensional parameters: the expectations, the average standard deviation and the probability of contact lines maximum data distributions background components and raw spectrogram peaks and intensities for fibers without nanoparticles and nanoparticles.

6. An assessment of the reliability of a multidimensional control of the presence of nanoparticles on polyethylene fiber for maximum probability of contact lines of data distributions background components and raw spectrograms and peak intensities for fibers without nanoparticles and nanoparticles.

7. Identified by mathematical models of the data reliability control of the presence of gold nanoparticles on the back-end components. The range of values of reliability varies from 0.9995 to peak with i = 0 to 0.9967 for the peak with i = 6. These values indicate a very high accuracy of the control of the presence of gold nanoparticles in the PE fibers.

8. Evaluation of the accuracy control of the presence of gold nanoparticles on the original spectrograms with the peaks and background components revealed a change in the value range of 0.9989 to the reliability of the peak with i = 0 to 0.9790 for the peak with i = 5. These values indicate a high accuracy control of the presence of gold nanoparticles with PE fibers.

9. Monitoring the availability of gold nanoparticles only on the peaks of the spectrograms without background components gives the low reliability. The range of values of reliability varies from 0.6915 to peak with i = 0 to 0.9262 for the peak with i = 1. These values indicate a very low reliability of the control of the presence of gold nanoparticles in the PE fibers.

10. Defined by generalized parameter values common to i = 0...6 distributions: evidence of generalized reliability of the control components for background on the original spectrograms, and only on the peaks: $P\xi v = 0.991546$, $P\xi w = 0.971375$, $P\xi s = 0.720666$. From these pooled data shows that the highest accuracy of the method has a control for background components, the accuracy and the lowest was obtained in the control on the spectrogram peaks without background components.

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