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Evaluation of Silver and Gold Nanoparticles on Polyester Fibers by Fluorescent Polarization Raman Spectra

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The results of the validation of identification nanoparticle colloidal silver and gold on the polyester fibers on the background component of the Raman spectra in the control based on the polarization characteristics. The accuracy of identification of nanoparticles was evaluated by the joint probability of crossing normal scatter intensity distributions Raman spectrograms as silver nanoparticles and gold nanoparticles on polyester fibers, depending on the longitudinal and transverse polarization of the laser radiation on the entire range of wave numbers. Defined generalized parameter values common to distributions over the entire range for each wave numbers with the polarization of the laser and across the grain, and generalized reliability of the control and identification of nanoparticles of silver, gold for assessing the likelihood of the complete group of events. Set the sensitivity of detection reliability.

Keywords: Polyester fiber, Colloidal nanoparticles of silver and gold, Raman spectra, Polarization characteristics of Raman spectroscopy, Mathematical modeling of the spectra, Background fluorescent components of the Raman spectra, Accuracy of control, Probability of crossing the scatter of normal distributions.

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1. INTRODUCTION

The polarization characteristics of the Raman scattering of light or Raman spectroscopy can significantly increase the accuracy of identification for control nanoparticles are on the fibers of textiles.

The work performed [1-6] allow us to estimate the presence of nanoparticles on polyester fibers, but define them as belonging to the silver or gold is difficult because of their small number. Increase the reliability of the use of multivariate methods allow estimation of reliability and vector-matrix correlation and autocorrelation polarization characteristics and components of the Raman spectra.

2. DESCRIPTION OF THE SUBJECT AND METHODS OF RESEARCH

2.1 Experimental Procedure

In the experiment are chosen polyester (PE) fibers, which were deposited on silver nanoparticles colloidal solution of silver nano AgBion-2 (TU 2499-003-44471019-2006 Concern "Nanoindustry") and colloidal gold nanoparticle solution of gold nanoparticles (TU 9154-001-93099853-06 NGOs Biotest). Of textile materials nanoparticles was carried out in the laboratory of the Chemistry Department of Southwest State University. Polyester fiber was chosen because of the small number of peaks – the main components of the Raman spectrum. As a result, there were obtained:

– samples with silver nanoparticles measured with polarization along the fiber 1Ag, 2Ag and 3Ag; samples 4Ag, 5Ag and 6Ag - with silver nanoparticles measured with polarization perpendicular to the grain;

– samples with gold nanoparticles measured with polarization along the fibers 1Au, 2Au and 3Au; and samples with gold nanoparticles 4Au, 5Au and 6Au measured with polarization perpendicular to the grain. The measurements were performed with a scanning probe microscope (SPM) with a confocal Raman and fluorescence spectrometer OmegaScope ™. On each sample were measured with the polarization of the laser beam and across the grain at the location of the fibers with the stage on the table microscope SPM.

2.2 The Processing of the Experimental Data

Translation Raman spectrograms of the program was carried out in Mathcad Spekwin32 through Excel compatible ASCII. As a result, the spectrograms were obtained polyester fibers E1Ag, E2Ag, E3Ag, E4Ag, E5Ag, E6Ag with silver nanoparticles and E1Au, E2Au, E3Au, E4Au, E5Au, E6Au with gold nanoparticles. The next step performed mathematical modeling background constituents from the separation in accordance with the procedure described in [1]. As a result, the values of background components A1 (X1), A2 (A2), A3 (A3), A4 (X4), A5 (X5), A6 (X6) for fibers with silver nanoparticles and A1Au (XAu1), A2Au (XAu2), A3Au (XAu3), A4Au (XAu4), A5Au (XAu5), A6Au (XAu6) for fibers with gold nanoparticles. Fig. 1 and 2 show the spectrograms obtained for samples 1Ag, 4Ag, 1Au, 4Au.

Estimation of parameters of the intensity distribution of the spectrograms of Fig. 1-2 performed using the program Mathcad. Respectively, were determined expectations spectra intensities nanochatsitsami silver fibers: ME123Agi, ME456Agi and gold nanoparticles: ME123Aui, ME456Aui, and standard deviations, respectively: $\sigma\Delta123Agi$, $\sigma\Delta456Agi$, $\sigma\Delta123Aui$, $\sigma\Delta456$ Aui.

To quantify the differences you need to consider the accuracy of the control lines on the probability of contact with tolerances coefficient yi: ME123i-yi·σΔ123i and

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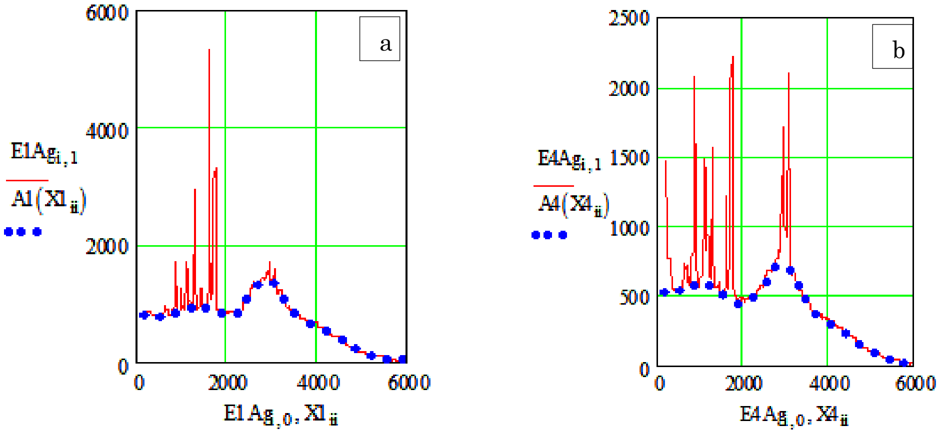


Fig. 1 – Spectrogram Raman Raman scattering and background fluorescent components in the system MathCad: a – polarization along the PE fibers with silver nanoparticles; b – polarization across PE fibers with silver nanoparticles

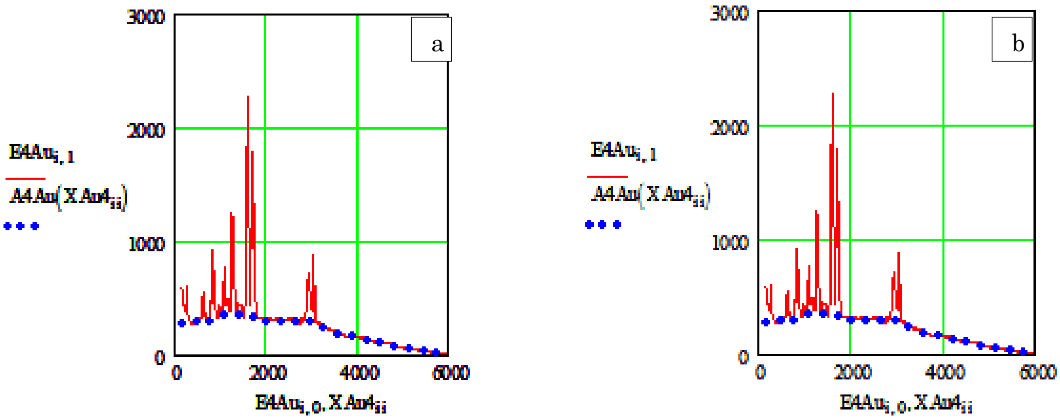


Fig. 1 – Spectrogram Raman Raman scattering and background fluorescent components in the system MathCad: a – polarization along the PE fibers with gold nanoparticles; b – polarization across PE fibers with gold nanoparticles

ME456i-yi·σΔ456i, as well as for ME123Aui-yAui·σΔ123Aui and ME456Aui-yAui·σΔ456Aui, and combinations thereof. Contact lines detected in the simulation by determining the coefficients yi, so that the lines touch at one point for each of i = 0 ... n:

$y_i := (ME123Ag_i - ME456Ag_i) / (\sigma\Delta456Ag_i + \sigma\Delta123Ag_i)$,
$yAu_i := (ME123Au_i - ME456Au_i)/(\sigma\Delta456Au_i + \sigma\Delta123Au_i)$,
$y123AgAu_i := (ME123Ag_i ME123Au_i) / (\sigma\Delta123Ag_i + \sigma\Delta123Au_i)$,
$y456AgAu_i := (ME456Au_i - ME456Ag_i) / (\sigma\Delta456Au_i + \sigma\Delta456Ag_i)$, (1)
$y16_i := (ME123Ag_i - ME456Au_i)/(\sigma\Delta456Au_i + \sigma\Delta123Ag_i)$ (1)

Estimation of reliability for silver nanoparticles carried by the following expressions:

$p1_i = 1 - pnorm(ME123Ag_i - y_i \,.\, \sigma\Delta123Ag_i,\ ME123Ag_i,\ \sigma\Delta123Ag_i)$,
$p2_i = pnorm(ME456Ag_i + y_i . \sigma\Delta456Ag_i,\ ME456Ag_i,\ \sigma\Delta456Ag_i)$. (2)

By equations (3) is estimated for the accuracy of the gold nanoparticles:

$p1Au_i = 1 - pnorm(ME123Au_i - yAu_i \cdot \sigma\Delta123Au_i,\ ME123Au_i,\ \sigma\Delta123Au_i)$,
$p2Au_i = pnorm(ME456Au_i + yAu_i \cdot \sigma\Delta456Au_i,\ ME456Au_i,\ \sigma\Delta456Au_i)$. (3)

Together silver and gold nanoparticles for polarization along the fiber is estimated accuracy of the following expressions:

$p1123AgAu_i = 1 - pnorm(ME123Ag_i - y123AgAu_i \cdot \sigma\Delta123Ag_i,\ ME123Ag_i,\ \sigma\Delta123Ag_i)$,
$p2123AgAu_i = pnorm(ME123Au_i + y123AgAu_i . \sigma\Delta123Au_i,\ ME123Au_i \sigma\Delta123Au_i)$. (4)

Equations (5) the accuracy of the estimated together silver and gold nanoparticles with polarization perpendicular to the grain:

$p1456AgAu_i = 1 - pnorm(ME456Au_i - y456AgAu_i \cdot \sigma\Delta456Au_i,\ ME456Au_i,\ \sigma\Delta456Au_i)$,
$p2456AgAu_i = pnorm(ME456Ag_i + y456AgAu_i \cdot \sigma\Delta456Ag_i,\ ME456Ag_i,\ \sigma\Delta456Ag_i)$. (5)

Silver nanoparticles together with polarization along the fibers and gold nanoparticles with polarization perpendicular to the grain is estimated accuracy of the following:

$p116AgAu_i = 1 - pnorm(ME123Ag_i - y16_i \cdot \sigma\Delta123Ag_i,\ ME123Ag_i,\ \sigma\Delta123Ag_i)$,
$p216AgAu_i = pnorm(ME456Au_i + y16_i \cdot \sigma\Delta456Au_i,\ ME456Au_i,\ \sigma\Delta456Au_i)$. (6)

3. DESCRIPTION AND ANALYSIS OF RESULTS

Determine the reliability of the results from the expressions (1) - (6) are shown in Figure 3-4.

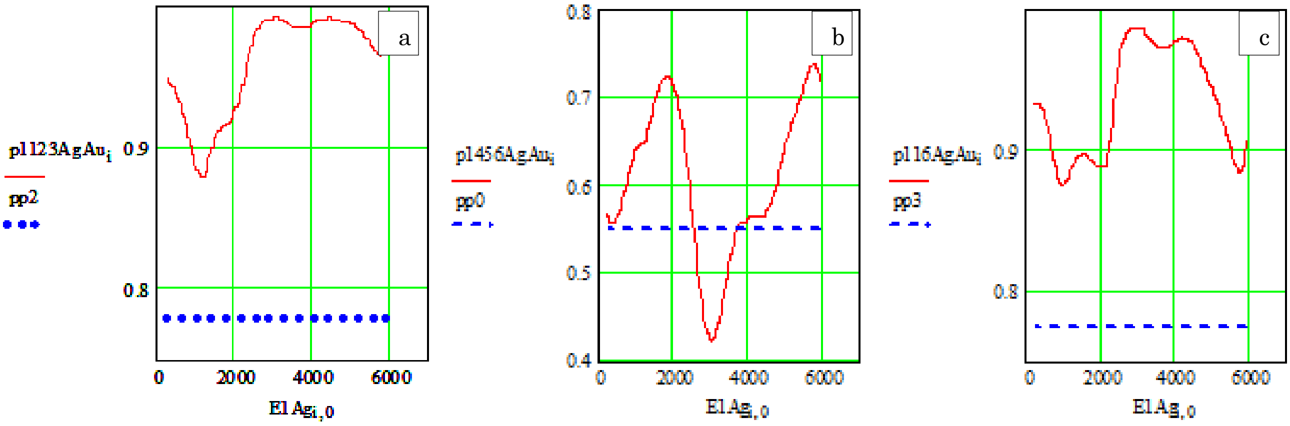


Fig. 3 – The accuracy of identification when joint control presence of nanoparticles of silver and gold: a – silver and gold nanoparticles for polarization along the fiber; b – silver and gold nanoparticles with polarization perpendicular to the grain; c - silver nanoparticles for polarization along the fibers and gold nanoparticles with polarization perpendicular to the grain

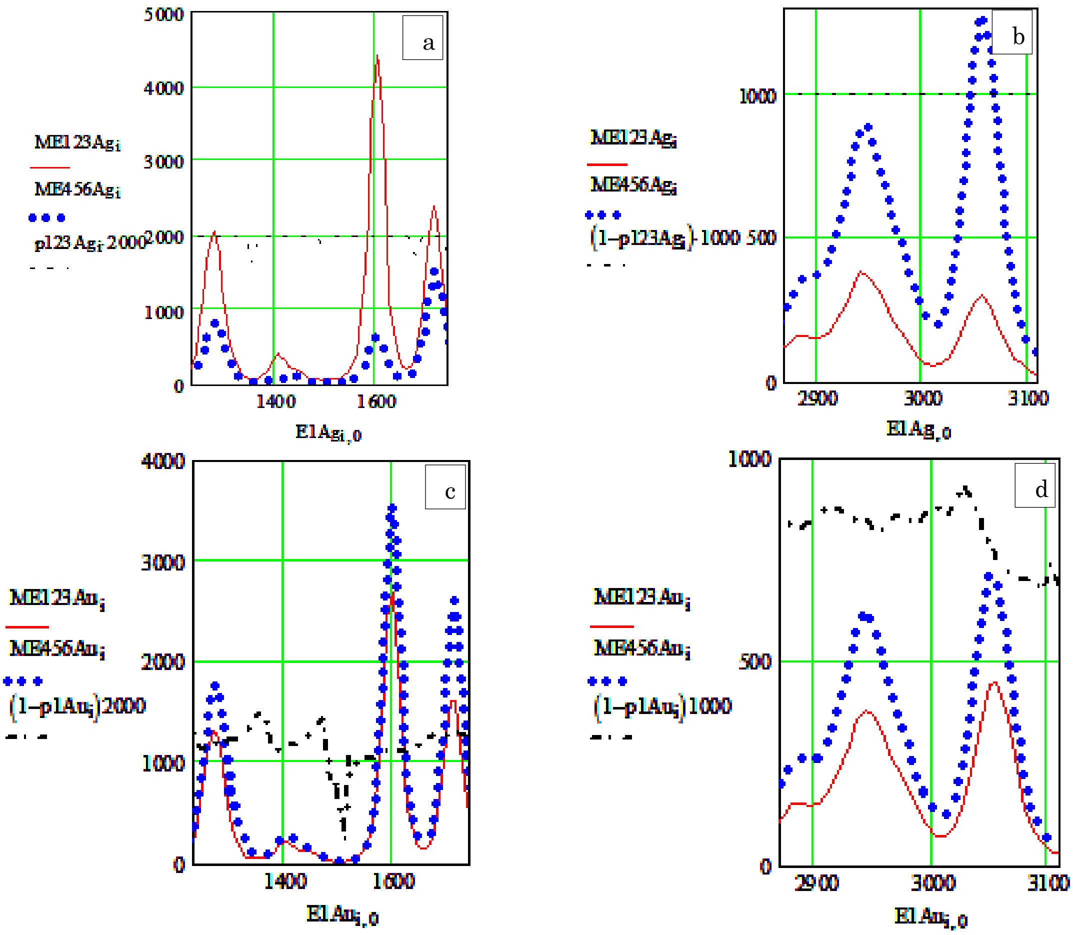


Fig. 4 – Reliability of identifying the presence of nanoparticles in the control of silver and gold in the local areas of the range of wave numbers: a - silver nanoparticles for polarization along and across the grain in the range of wave numbers E1Agi, 0 = 1240 ÷ 1740 cm -1; b - silver nanoparticles for polarization along and across the grain in the range of wave numbers E1Agi, 0 = 2870 ÷ 3110 cm-1; c - gold nanoparticles for polarization along and across the grain in the range of wave numbers E1Agi, 0 = 1240 ÷ 1740 cm -1; d - gold nanoparticles for polarization along and across the grain in the range of wave numbers E1Agi, 0 = 2870 ÷ 3110 cm-1

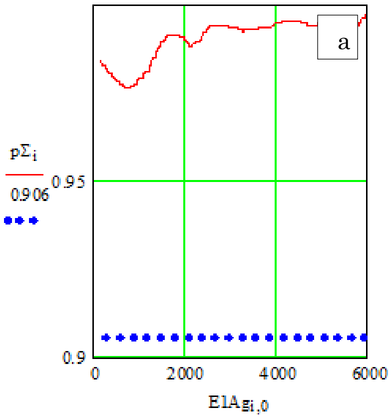
The accuracy of the identification of silver and gold nanoparticles with control showed high values in local areas of the range of wave numbers up to 0.994. However, the accuracy of the identification of silver and gold nanoparticles with control on the mean intensity spectrograms simultaneously across the entire range of wave numbers gives lower values: p1_0=0.813, p1Au_0=0.499, p1123AgAu_0=0.777, p1456AgAu_0=0.551, pp116AgAu_0= 0.774.

Therefore, it was simulated authenticity identification of silver and gold nanoparticles by assessing the likelihood of the complete group of events:

$p\Sigma_i$ = 1- (1 – p123Ag_i) (1 – p1Au_i), min($p\Sigma_i$) = 0.976, max($p\Sigma_i$) = 0.997;

$p\Sigma 0=1-(1-0.813)\cdot(1–0.5), \quad p\Sigma 0=0.906.$ (7)

The results of the validation by model (7) are shown in Figure 5.



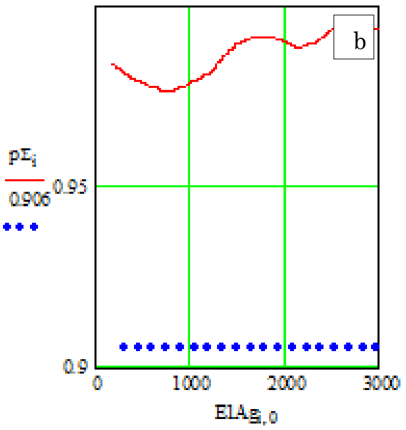


Fig. 5 – Authenticity of identification with the joint control of nanoparticles of silver and gold on a full assessment of the probability of an event group: a - normal scale of spectrogram reliability; b - zoomed spectrogram reliability

Therefore, the accuracy of identification was evaluated nanoparticles of silver and gold on local areas and peaks (Table 1).

For wavenumbers E1$Ag_{i,0}$ = 1240 ÷ 1740 cm^{-1} fibers with silver nanoparticles the accuracy of the identification of high p123Agi = 1.000 when compared to the longitudinal and transverse ME123Agi ME456Agi components because the longitudinal component ME123Agi intensity much more transverse ME456Agi, and the average standard deviation σΔ123Agi 50 times less ME123Agi.

In the region of wave numbers E1$Ag_{i,0}$ = 2870 ÷ 3110 cm^{-1} for silver nanoparticles the accuracy of the identification of high 1 - p123Agi = 1.000 (p123Agi = 0.000) between the transverse and longitudinal ME456Agi ME123Agi components, due to the fact that the transverse component ME456Agi intensity much more longitudinal ME123Agi. Standard deviation σΔ123Agi 10 times less ME123Agi.

For gold nanoparticles in the region of wave numbers E1$Au_{i,0}$ = 1240 ÷ 1740 cm^{-1} identification accuracy of the lowest p1Aui <0.500 when assessing longitudinal and transverse ME123Aui ME456Aui components. This is due to the fact that the transverse component ME456Aui intensity slightly more longitudinal ME123Aui, and the average standard deviation σΔ123Aui comparable ME123Aui.

The accuracy of identification for gold nanoparticles is not very high 1 - p123Aui ≈ 0.800 (p123Aui ≈ 0.200) with the transverse and longitudinal ME456Aui ME123Aui components in the wave-number E1Aui, 0 = 2870 ÷ 3110 cm-1 due to the fact that the transverse component ME456Aui intensity a little more longitudinal ME123Aui, and standard deviations σΔ123Aui less ME123Aui.

Data reliability of the control and proxy authentication nanoparticles of silver and gold, identified by mathematical models (1-6) are in the range of from 0.2 to 0.997 over the entire range for each wave numbers with the polarization of the laser and across the grain . It shows high sensitivity detection reliability .According to the model (7) are defined generalized parameter values common to distributions over the entire range for each wave numbers, and generalized reliability of the control and identification of nanoparticles of silver and gold on a full assessment of the probability of an event group . In this case, the validity range is changed from a minimum value 0.976 to a maximum 0.997. The accuracy of the identification of silver and gold nanoparticles with control on the mean intensity spectrograms simultaneously across the entire range of wave numbers, taking into account estimates of the probability of the complete group of events (7) gives a high confidence value 0.906.

4. CONCLUSIONS

1. Due to the large scatter in the values of parameters in the control information of silver and gold nanoparticles on polyester fibers and considerable uncertainty in the laws of their manifestation of the most highly reliable control of the presence of nanoparticles and their identification method of accounting gives the polarization of the laser radiation and across the grain with the identification of background fluorescent components.

Table 1 - Reliability of identification of nanoparticles under control by peaks

E1$Ag_{i,0}$	861.11	999.30	1091.0	1176.0	1283.0	1406.0	1598.0	1713.0	2949.0	3057.0
ME123Ag_i	882.97	391.68	844.46	166.01	2046.0	360.77	4435.0	2386.0	364.22	298.02
ME456Ag_i	1265.00	37.969	735.91	307.89	841.05	71.191	639.42	1521.0	878.95	1280.0
p123Ag_i	0.0455	1.000	0.784	0.009	1.000	1.000	1.000	1.000	0.000	0.000
ME123Au_i	762.09	190.26	600.24	133.79	1253.0	212.85	2696.0	1617.0	365.30	450.17
ME456Au_i	1132.00	297.99	844.46	261.58	1776.0	296.45	3556.0	2615.0	574.41	699.90
p1Au_i	0.316	0.409	0.355	0.192	0.410	0.426	0.436	0.358	0.178	0.225

2. A method for determining the reliability of the control of nanoparticles to determine the parameters of the laws of the intensity distribution of the Raman spectrum for each value in the whole range of wave numbers for spektogramm at polyaizatsii laser radiation along and across fibers containing nanoparticles of silver and gold.
3. To improve the reliability of identification of silver and gold nanoparticles on the fibers of the mathematical modeling of data spectrograms their generalized mathematical expectations and generalized standard deviation , as well as generalized probabilities of contact lines of distribution is spectrograms.
4. To eliminate uncertainty and identify patterns in the distribution of the parameters evaluated spectrograms joint parameters spectrograms intensities depending on the wave number (frequency) components as spectrograms with laser radiation along the grain and across the nanoparticles in the presence of silver and gold.
5. Estimated multidimensional parameters : the expectations , the average standard deviation of the spectral components of the fiber with silver and gold nanoparticles in the laser polarization and across the grain.
6. Evaluation of multivariate testing reliability and indetifikatsii nanoparticles on polyester fibers for maximum probability of contact lines of data distributions and spectrograms components peaks intensities for fibers with silver and gold nanoparticles in the laser polarization and across the grain.
7. Revealed by mathematical models of control and data reliability of proxy authentication silver and gold nanoparticles in the range of 0.2 to 0.999 over the entire range for each wave numbers with the polarization of the laser and across the grain, which indicates a high sensitivity of the method.
8. Reliable identification of nanoparticles of silver and gold at the control on the mean intensity spectrograms simultaneously across the entire range of wave numbers gives lower values: p1_0=0.813, p1Au_0=0.499, p1123AgAu_0=0.777, p1456AgAu_0=0.551, pp116AgAu_0= 0.774.
9. Processing mathematical models of control and identification of nanoparticles of silver and gold with generalized parameter values for the distributions of the mean intensity spectrograms simultaneously across the entire range of wave numbers when assessing the likelihood of the complete group of events gives the value generalized reliability 0.906. This value indicates the high reliability of the control and identification of nanoparticles of gold and silver on polyester fibers.
10. Determined by generalized parameter values common to distributions over the entire range for each wave numbers, and generalized reliabilities control on reliability of identification of silver and gold nanoparticles in assessing the likelihood of the complete group of events. The range of values of reliability varies from a minimum of 0.976 to a maximum of 0.997.

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