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Development of a Technique of an Analytical Assessment of Crossing of Ellipses of Distribution on Polarizing Raman Ranges at Identification of Nanoparticles of Silver on Polyester Fibers

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Analytical estimates of crossing of ellipses of distribution at recognition of nanoparticles of colloidal silver are given in polyair fibers on multidimensional correlation components of the Raman ranges with control according to polarizing characteristics. Reliability of recognition of nanoparticles was estimated on joint probability of normal distributions of intensivnost of the Raman spectrograms of nanoparticles of silver on polyair fibers depending on longitudinal and cross polarization of laser radiation on all range of a range with the analysis of 9 main peaks.

Keywords: Polyester fiber, Nanoparticles of colloidal silver, The Raman ranges, Polarizing characteristics of the Raman spectroscopy, Mathematical modeling of ranges, Multidimensional correlation components of the Raman ranges, Reliability of recognition.

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1. INTRODUCTION

Correlation polarizing characteristics of the Raman spectroscopy allow to increase considerably reliability of recognition of the nanoparticles which are on fibers of fabrics.

In works [1-7] identification of nanoparticles on polyair fibers is estimated. But to define the modes of drawing nanoparticles on fibers and especially their change at operation it is complicated because of their small quantity.

The offered researches allow to increase the accuracy of recognition of the fibers covered with nanoparticles of silver or uncovered nanoparticles according to polarizing characteristics of the Raman ranges with use of methods of an analytical assessment of crossing of ellipses of distribution of intensity of polarizing Raman ranges.

2. DESCRIPTION OF THE SUBJECT AND METHODS OF RESEARCH

2.1 Experimental Procedure

Experiments on measurement of casual values of distribution of intensivnost of ranges of the Raman combinational radiation were previously made, thus correlation matrixes (Fig. 1) and parameters of distributions (1) taking into account polarization of radiation on X-across and on Y- along fibers at the same time for one measurement are revealed:

$$\mathrm{rXY1} := \begin{pmatrix} 0.97773 & 0.96578 & 0.98175 & 0.97934 & 0.98689 & 0.97556 & 0.98801 & 0.6027 & 0.7786 \\ 0.79865 & 0.76332 & 0.82619 & 0.79872 & 0.80578 & 0.79539 & 0.83044 & 0.24558 & 0.42347 \\ 0.96434 & 0.95148 & 0.95214 & 0.96733 & 0.97768 & 0.96159 & 0.96942 & 0.64528 & 0.82663 \\ 0.9752 & 0.96919 & 0.96496 & 0.97817 & 0.98874 & 0.97285 & 0.97782 & 0.67926 & 0.85655 \\ 0.97342 & 0.98244 & 0.97044 & 0.97551 & 0.98303 & 0.97247 & 0.97035 & 0.74055 & 0.89334 \\ 0.93736 & 0.91504 & 0.92737 & 0.94071 & 0.954 & 0.93365 & 0.94936 & 0.55032 & 0.74837 \\ 0.99096 & 0.98829 & 0.98601 & 0.9928 & 0.99868 & 0.98952 & 0.99209 & 0.71 & 0.87045 \\ 0.8729 & 0.88349 & 0.84044 & 0.87375 & 0.8666 & 0.87397 & 0.85002 & 0.88461 & 0.96211 \\ 0.93204 & 0.93567 & 0.91286 & 0.93657 & 0.95276 & 0.92941 & 0.92861 & 0.7075 & 0.88746 \end{pmatrix}$$

a

$$\mathrm{rXYAg9\_0\_8} := \begin{pmatrix} 0.552995 & 0.551386 & 0.584333 & 0.578084 & 0.812568 & 0.582131 & 0.810429 & 0.70569 & 0.701413 \\ 0.072707 & 0.059823 & 0.110294 & 0.096263 & 0.450515 & 0.102463 & 0.448721 & 0.328623 & 0.298 \\ 0.24972 & 0.243948 & 0.284734 & 0.276869 & 0.591059 & 0.289241 & 0.585284 & 0.459355 & 0.421098 \\ 0.423143 & 0.427049 & 0.456838 & 0.453528 & 0.711963 & 0.46017 & 0.70798 & 0.583401 & 0.574415 \\ -0.218246 & -0.196189 & -0.182804 & -0.177064 & 0.11285 & -0.169192 & 0.106614 & -0.055889 & -0.062892 \\ 0.498818 & 0.506106 & 0.531324 & 0.529385 & 0.75771 & 0.532267 & 0.755237 & 0.635997 & 0.642651 \\ -0.298202 & -0.276126 & -0.263092 & -0.257816 & 0.032243 & -0.251863 & 0.027018 & -0.13289 & -0.13578 \\ -0.340895 & -0.37365 & -0.319459 & -0.336261 & -0.005625 & -0.307772 & -0.016419 & -0.088009 & -0.209583 \\ -0.144616 & -0.137314 & -0.107137 & -0.110232 & 0.219236 & -0.103791 & 0.215268 & 0.06711 & 0.051273 \end{pmatrix}$$

b

Fig. 1 – Correlation matrixes of the Raman polarizing spectrograms of polyester fibers after drying under natural conditions in the range of frequencies 54.3÷3110 sm^{-1}: a – polarization across and along fibers with silver nanoparticles; b – polarization across and along fibers without silver nanoparticles

In Fig. 1 it is visible that korellyatsionny matrixes have the big range of dispersion of values from 0.99868 till 0.24558 in the presence of nanoparticles of silver (fig. 1a), and for fibers without nanoparticles range from 0.812568 to – 0.340895.

Parameters of distributions (1), and, population means considerably differ on intensity of peaks of ranges with polarization across fibers X and along fibers Y. Along fibers intensity is much higher even several times both for fibers without nanoparticles, and for fibers with nanoparticles.

Characteristic is that at polarization along fibers intensity of the central peaks 4, 5, 6 and 7 is much higher than extreme peaks 1, 2, 3, 8 and 9 almost by 20 times. It specifies that maximum efficiency of measurements of the Raman ranges at polarization along fibers is found. However there is a task about check of informational content at measurement of peaks of polarizing ranges of the Raman radiation.

MENX$^{\mathrm{T}}$ = (698.207 266.156 384.805 659.824 661.551 852.41 849.92 412.99 796.091),

σΔX$^{\mathrm{T}}$ = (84.487 50.527 47.174 73.693 77.891 89.624 87.343 16.679 31.712),

MENY$^{\mathrm{T}}$ = (745.167 457.096 1196.862 4023.730

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4073.140 1775.226 1780.878 182.674 196.222),

$\sigma\Delta Y^T$ = (115.383 74.971 626.399 571.34 270.561 255.402 29.143 15.207),

$MENXAg9^T$ = (395.233 140.846 213.373 332.365 344.734 478.977 510.665 270.979 539.491),

$\sigma\Delta YAg9^T$ = (60.722 35.107 27.743 40.744 55.448 46.836 65.423 24.641 50.471),

$MENYAg9^T$ = (599.064 365.357 968.096 3224.61 2929.766 1431.412 1342.996 136.366 150.694),

$\sigma\Delta YAg9^T$ = (120.429 74.806 195.827 612.321 706.978 273.100 321.016 32.870 29.676). (1)

2.2 The Processing of the Experimental Data

We will carry out modeling of statistical data for identification of crossings of ellipses of distributions of values of intensivnost of peaks of spectrograms. We will create the general correlation matrix for full generation of data on the basis of initial matrixes of Fig. 1 and we will receive a correlation matrix of RXY1 with a general size of 38 × 38.

Generation of the set amount of casual values is carried out in normal way to the law and a matrix of RXY1 for what the built-in MathCad Edition 14 [4-6] function is used. Further we define a vector of own numbers from the general correlation matrix of RXY1.

As the generated casual values possess some correlation which is negatively affecting modeling accuracy, it is necessary to lead them to an uncorrelated look for what the special program developed in the environment of MathCad Enterprise Edition 11 is used. The values of data of modeling received by such transformation possess the correlation aspiring to zero.

Further we will transform uncorrelated values through a fundamental matrix of UR of a correlation matrix of RXY1 to the correlated.

For automatic identification of crossing of ellipses of distribution it is necessary to solve system of the analytical equations and it will give coordinates of a point of intersection. In this work the system only of two equations is considered.

The analytical assessment of crossing of ellipses of distributions is made according to the decision of system of the equations with finding of coordinates of a point of intersection:

$rXY1_3 := 0.97817;$ $rXYAg9\_0\_8_3 := 0.453528;$

$f(x,y) := ((x-MENXAg9_3)/\sigma\Delta XAg9_3)^2 - 2\cdot rXYAg9\_0\_8_3\cdot((x-MENXAg9_3)/\sigma\Delta XAg9_3)\cdot((y-MENYAg9_3)/(\sigma\Delta YAg9_3) + ((y-MENYAg9_3)/\sigma\Delta YAg9_3)^2-4\cdot 3.201055\cdot[1-(rXYAg9\_0\_8_3)^2];$

$g(x,y):((x-MENX_3)/\sigma\Delta X_3)^2-2\cdot rXY1_3\cdot((x-MENX_3)/\sigma\Delta X_3)\cdot((y-MENY_3)/\sigma\Delta Y_3)+((y-MENY_3)/\sigma\Delta Y_3)^2-4\cdot 3.201055\cdot[1-(rXY1_3)^2];$

$x := 400$ $y := 2000$ $f(x,y) = 0$ $g(x,y) = 0$

$v := Find(x,y)$

$v = (405.701697, 2036.720505)$

$f(v_0, v_1) = 7.127\cdot 10^{-5}$

$g(v_0, v_1) = 9.997\cdot 10^{-4}.$ (2)

The decision of system of the analytical equations (2) is made by criterion of crossing of ellipses not in two points, and in one for coordinates of limit values X0(1) = 485.948874 and X0(2) = 485.948889 for Ro2 = 4·1.7321043. For double crossing of ellipses of distribution the transition point from one crossing is revealed (only contact) $R_o^2 = 4\cdot 1.733$ $X_0 = 486.01424$.

For coordinate $Y_{0(1)} = 481.103016$ and $Y_{0(2)} = 481.103048$ for $R_o^2 = 4\cdot 1.7321043$ limit value of crossing is revealed. At the beginning of double crossing the transition point from one point of intersection is revealed $R_o^2 = 4\cdot 1.733$ $Y_0 = 481.16753$.

Coordinates of limit values $X_{3(1)} = 485.948874$ and $X_{3(2)} = 485.948889$ for $R_3^2 = 4\cdot 1.7321043$. For double crossing of ellipses of distribution the transition point from one crossing is revealed (only contact) $R_3^2 = 4\cdot 3.2027$ $X_3 = 405.766908$.

For coordinate $Y_{3(1)} = 2036.720524$ and $Y_{3(2)} = 2036.720505$ for $R_3^2 = 4\cdot 3.201055$ limit value of crossing is revealed. At the beginning of double crossing the transition point from one point of intersection is revealed $R_3^2 = 4\cdot 3.2027$ $Y_3 = 2037.098168$.

3. DESCRIPTION AND ANALYSIS OF RESULTS

At an analytical assessment of crossing of ellipses of distribution with the decision of system of the equations coordinates on 9 peaks are received:

for cross polarization of X

XAn^T = (485.949 192.204 267.401 405.702 474.262 566.027 653.626 349.531 695.899) (3)

for longitudinal polarization of Y

YAn^T = (481.103 373.014 771.483 2036.72 2729.72 1061.13 1212.73 105.587 153.743) (4)

and the equivalent radius of curvature of ellipses when crossing

RAn^T = (2.632 1.463 2.537 3.578 2.399 3.336 2.234 3.255 3.159) (5)

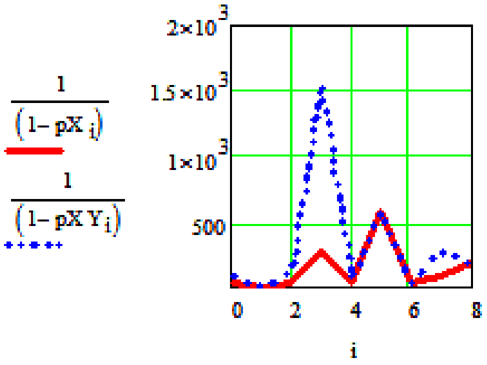

Fig. 2 – Increase of informational content of reliability when using two-dimensional measurement in cross X and longitudinal At the directions taking into account correlation coefficients: __ measurements at cross polarization of X; …. measurements in cross X and longitudinal At the directions taking into account correlation coefficients

In comparison with experimental data when modeling with use of generation of multidimensional correlation dependences of coordinate of crossing of ellipses of distribution following:

for cross polarization of X

$XЭn^T$ = (508.31 187.17 269.05 401.42 477.04 551.12 670.90 334.39 712.03) (6)

for longitudinal polarization of Y

$$YЭn^{T} = (590.97 \quad 558.13 \quad 827.27 \quad 2005.9 \quad 2945.7 \quad 1138.8 \quad 1318.1 \quad 133.93 \quad 166.18) \qquad (7)$$

At a choice of points of intersection of the ellipses of distribution constructed on population means, average quadratic deviations and correlation coefficients with selection of equivalent radius of ellipses of distribution crossing coordinates are received:

for cross polarization of X

$$XPn^{T} = (488.20 \quad 192.22 \quad 267.37 \quad 409.82 \quad 474.45 \quad 565.68 \quad 654.19 \quad 349.52 \quad 697.07) \qquad (8)$$

for longitudinal polarization of Y

$$YPn^{T} = (486.00 \quad 373.44 \quad 770.96 \quad 2095.7 \quad 2731.2 \quad 1059.1 \quad 1214.3 \quad 105.60 \quad 154.13) \qquad (9)$$

and the equivalent radius of curvature of ellipses when crossing

$$RPn^{T} = (2.636 \quad 1.463 \quad 2.538 \quad 3.584 \quad 2.403 \quad 3.335 \quad 2.241 \quad 3.255 \quad 3.122). \qquad (10)$$

4. CONCLUSIONS

The method giving substantial increase estimates reliability of definition of the modes of drawing nano-particles of silver on fibers that illustrates Fig. 2 was as a result offered.

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