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Development of Two-dimensional Analytical Model According to Polarizing Characteristics of the Raman Ranges at Recognition of Nanoparticles of Silver on Polyester Fibers

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Parameters of two-dimensional analytical model of an assessment 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 increased more than by 1000 times and 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, Two-dimensional correlation components of the Raman ranges, Reliability of recognition.

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1. INTRODUCTION

Considerably to increase reliability of recognition of the nanoparticles which are on fibers of fabrics correlation polarizing characteristics of the Raman spectroscopy due to multidimensional identification of a large number of peaks on the spectrogram allow.

The one-dimensional assessment of identification of nanoparticles on fibers of polyair is carried out in works [1-7]. But to define the modes of drawing nanoparticles on fibers and especially their change at operation is complicated because of their small quantity.

Carrying out statistical modeling of correlation parameters of intensity of ranges of fiber with silver nanoparticles during operation on analytical expressions of correlation ellipses of interdependent parameters with determination of coordinates of crossing represents considerable interest, and also an assessment of reliability of recognition of nanoparticles of silver.

2. DESCRIPTION OF THE SUBJECT AND METHODS OF RESEARCH

2.1 Experimental Procedure

We will carry out mathematical modeling of statistical data for identification of crossings of ellipses of distributions of values of intensivnost of peaks of spectrograms by the following technique [3]. We will create the general correlation matrix for full generation of data on the basis of initial matrixes and we will receive a correlation matrix of RXY1 with a general size of 38 × 38.

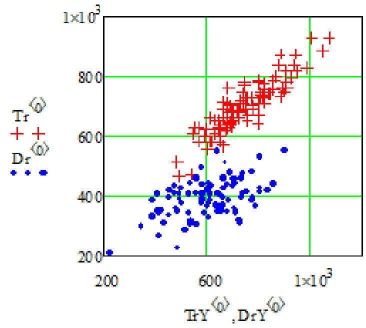
Generation of the set amount of casual values is carried out in normal way to the law and a matrix of RXY1 for what the built-in MathCad Edition 14 [3-5] function is used. Further we define a vector of own numbers from the general correlation matrix of RXY1.

As the generated casual values of a vector of own numbers 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 by authors in the environment of MathCad Enterprise Edition 11 is used.

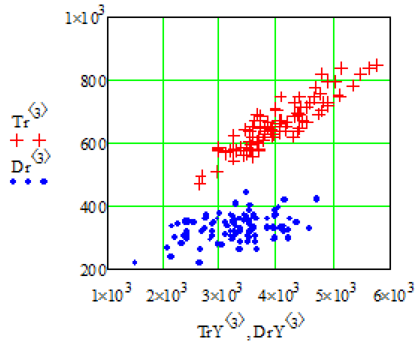
Further transformation of uncorrelated values through a fundamental matrix of UR of a correlation matrix of RXY1 in the correlated follows.

2.2 The Processing of the Experimental Data

The generated 96 values of data for 1 peak on an axis *X* and *Y* are given in Fig. 1a, and for 4 peaks in Fig. 1b.



a



b

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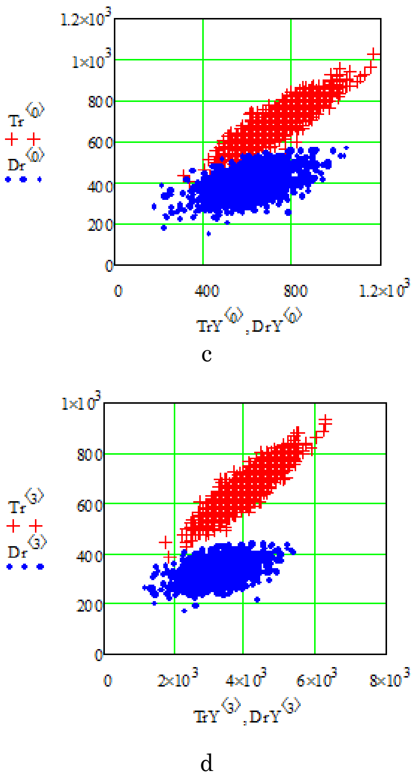

Fig. 1 – Two-dimensional correlation dependences of the Raman polarizing spectrograms of polyester fibers with nanoparticles of silver and without nanoparticles at polarization across and along fibers: a, b – a general view at generation of $n = 96$ of data for 1 and 4 peaks; c, d – a general view at generation of $n = 1536$ of data for 1 and 4 peaks

As data of Fig. 1a are crossed, it is possible to find a point of intersection easily. According to Fig. 1b it is visible that ellipses of distribution aren't crossed.

Therefore it is necessary to generate bigger number of data. 1536 generated data are given in Fig. 1c and 1d. On them it is visible that ellipses of 1 peak are crossed with considerable overlapping, and distribution ellipses 4 peaks are crossed normally.

Crossings of analytical ellipses of distribution of these peaks of spectrograms are given in Fig. 2. These ellipses are constructed on analytical mathematical expressions with parameters of population means, average quadratic deviations and coefficients of correlation for polyair fibers without nanoparticles (a continuous curve) and with nanoparticles (a curve points). For convenience of construction these drawings are developed on 180° round axis X in comparison with Fig. 1.

3. DESCRIPTION AND ANALYSIS OF RESULTS

Crossing happens in Fig. 2a, b $X1 = 488.2$ and $Y1 = 485.9$, and Fig. 2c, d of $X4 = 409.79$ and $Y4 = 2094.9$.

Crossings of ellipses of distribution on Fig. 1 find manually with number of the generated data. On Fig. 2 crossing are allocated with use of analytical mathematical expressions also manually at selection of the generalized R ellipse parameter – the equivalent radius of curvature.

For mathematical identification of crossing it is necessary to create system of the analytical equations

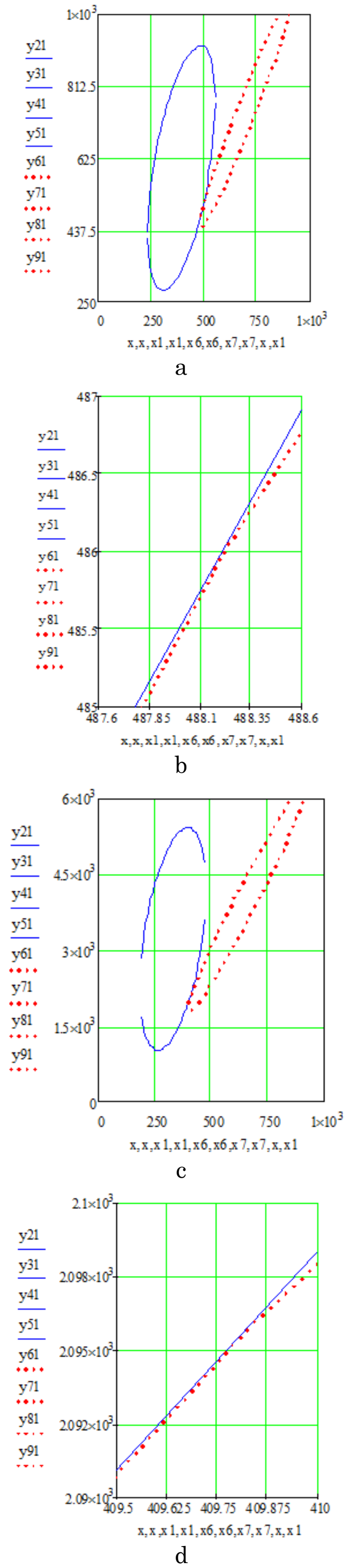

Fig. 2 – Crossing of ellipses of distribution at a task on analytical expressions (a continuous curve – without nanosilver; a curve with points – with nanosilver): a – a general view for 1 peak; b – the increased fragment with crossing of ellipses of distribution of 1 peak; c – a general view for 4 peaks; d – the increased fragment with crossing of ellipses of distribution 4 peaks

and it will give coordinates of a point of intersection.

The analytical assessment of crossing of ellipses of distributions is made on systems of the equations with finding of coordinates of a point of intersection (1)-(2):

$$iii := 0\ldots50 \quad x_{iii} := 10\cdot iii + MENXAg9_0;$$
$$x1_{iii} := -10\cdot iii + MENXAg9_0;$$
$$x6_{iii} := 10\cdot iii + MENX_0;\ x7_{iii} := -10\cdot iii + MENX_0. \quad (1)$$

$$y21_{iii} := 0.5\cdot\sigma\Delta YAg9_0\cdot[2\cdot rXYAg\_0\_8_0\cdot(x_{iii}-MENXAg9_0)/\sigma\Delta XAg9_0] + 0.5\cdot\sigma\Delta YAg9_0\cdot\{[2\cdot rXYAg9\_0\_8_0\cdot(x_{iii}-MENXAg9_0)/\sigma\Delta XAg9_0]^2-4\cdot[((x_{iii}-MENXAg9_0)/\sigma\Delta XAg9_0)^2-[1-(rXYAg\_0\_8_0)^2]\cdot 12.847]\}^{0.5} + MENYAg9_0; \quad (2)$$

The analytical equations for points are similarly received: y31iii, y41iii, y51iii, y61iii, y71iii, y81iii, y91iii.

Calculations on analytical expressions it is made by criterion of crossing of ellipses in one point (only contact) for coordinates of limit values $R1_{14} = 2.6355$ and $X1_{14} = 488.21$ on 1 peak of the spectrogram. For double crossing of ellipses of distribution points of intersection with results are revealed $Z1_{i,1} = X1_{i(1)} = 485.21\div503$ and $Z1_{i,3} = X1_{i(2)} = 488.21\div473$ at change $Z1_{i,0} = R_{1i} = 2.6355\div2.6739$.

For longitudinal polarization at $R1_{14} = 2.6355$ limit value of crossing is revealed $Y1_{14} = 485.98$. This beginning of double crossing of ellipses of distribution $Z1_{i,2} = Y1_{i(1)} = 485.98\div517$ and $Z1_{i,4} = Y1_{i(2)} = 485.98\div450$ at change of equivalent radius of an ellipse $Z1_{i,0} = R1_i = 2.6355\div2.6739$ on Fig. 3b.

Calculations on analytical expressions for 4 peaks it is shown on in Fig. 3c and 3d. Coordinates of limit values $R4_{14} = 3.58427$ and $X4_{14} = 409.81$ only contacts are received in a point. $X3_{(1)} = 485.948874$ and $X3_{(2)} = 485.948889$ for $R4 = 4\cdot1.7321043$. For double crossing of ellipses of distribution points are revealed $Z4_{i,1} = X4_{i(1)} = 409.81\div412$ and $Z4_{i,3} = X4_{i(2)} = 409.8\div400.5$ at change $Z4_{i,0} = R4_i = 3.58427\div3.58887$ on Fig. 3c.

For coordinate $Y4_{14} = 2095.4$ at $R4_{14} = 3.58427$ limit value of crossing is revealed. Double crossing happens in points of Fig. 3g and results of the decision $Z4_{i,2} = Y4_{i(1)} = 2095.4\div2125$ and $Z4_{i,4} = Y4_{i(2)} = 2095.3\div1960$.

4. CONCLUSIONS

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.

It is revealed that the closest compliance takes place at estimates XAn, Yan, Ran и XPn, YPn, RPn in comparison with the experimental XЭn, YЭn, where to estimate the equivalent radius of curvature of ellipses it wasn't presented possible in general. At an assessment of reliability of identification of nanosilver on fibers of polyair the following values for one-dimensional measurements on axis X in the cross direction of fiber are revealed:

for cross polarization of X

$$pX^T = (0.97917\ \ 0.92208\ \ 0.97917\ \ 0.99653\ \ 0.97917\ \ 0.99826\ \ 0.97917\ \ 0.98958\ \ 0.99479), \quad (3)$$

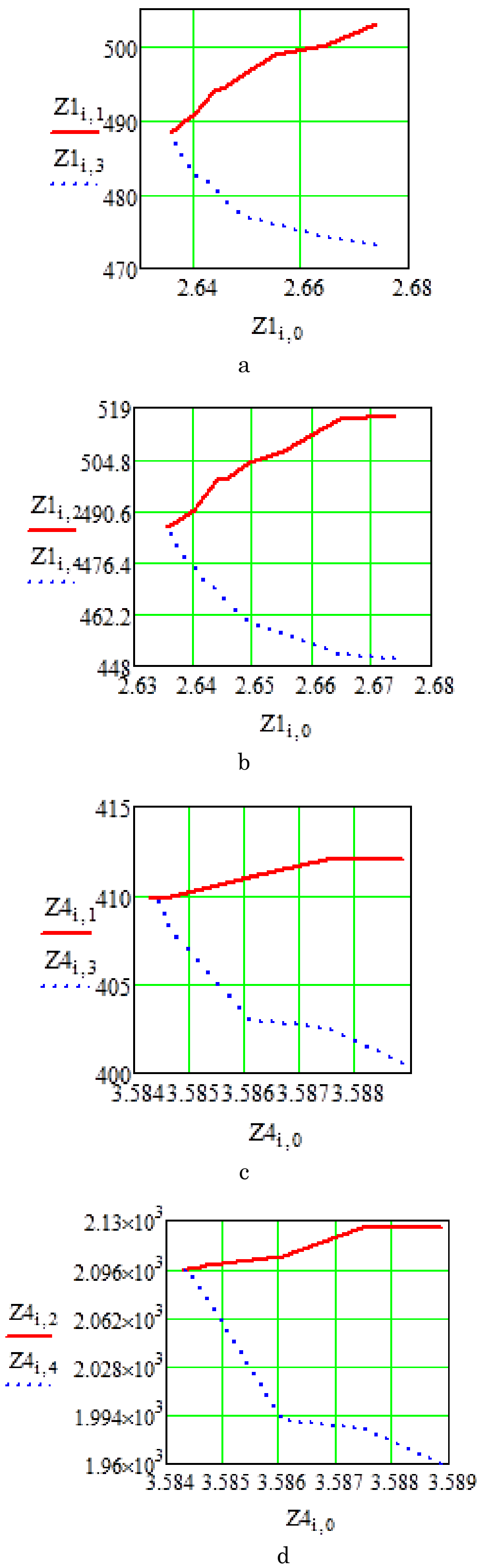

Fig. 3 – Images of crossings of ellipses of distribution on analytical expressions: a, b – a look when crossing $X1_{i(1)}$, $X1_{i(2)}$ and $Y1_{i(1)}$, $Y1_{i(2)}$; c, d – a look when crossing $X4_{i(1)}$, $X4_{i(2)}$ and $Y4_{i(1)}$, $Y4_{i(2)}$

for longitudinal polarization of Y

$$pY^T = (0.78125\ \ 0.70833\ \ 0.77083\ \ 0.81250\ \ 0.77083\ \ 0.72917\ \ 0.79167\ \ 0.72917\ \ 0.87500), \quad (4)$$

and at two-dimensional measurement in cross X and longitudinal Y directions taking into account correlation coefficients:

pXY^T = (0.9896 0.92708 0.99306 0.99935 0.98611 0.99826 0.97917 0.99653 0.99479). (5)

Here it is visible that the offered method gives an essential prize in an assessment of reliability of definition of the modes of drawing nanoparticles of silver on fibers. For example, for 4 peaks of i=3 the increase occurred more than by 1000 times.

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