Solution of system of multidimensional differential equations in X for identification of gold nanoparticles on fibers with elimination of uncertainty

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Abstract. There are the results of the compilation and solution of a system of multidimensional differential correlation equations of distribution ellipses in the identification of colloidal gold nanoparticles on polyester fibers with multi-dimensional correlation components of Raman polarization spectra. A proposed method is to increase the accuracy and speed of identification of silver nanoparticles on polyester fibers, taking into account the longitudinal and transverse polarization of laser radiation over the entire spectral range, analyzing in sequence and in order simultaneously two peaks along the X-transverse and along the Y-along the fibers. During a solution of the system using a nonlinear quadratic and differential equation with respect to X, an uncertainty arises, the elimination of which is numerical addition ∆ = + 0.02985

1. Introduction

To identify nanoparticles on the surface of materials, the most effective method is Raman spectroscopy, which provides a giant Raman scattering of light and makes it possible to increase the sensitivity for the recognition of metal nanoparticles by a factor of $10^7$ [1-3].

Identification of nanoparticles on polyester fibers is given in (research) [4, 5]. But these methods do not provide sufficient accuracy of the solution and automatically do not allow solving the system of equations in determining the modes of applying nanoparticles to fibers and especially the change in the number of particles during operation. Because of the great complexity of manual preparation and the selection of values for the equivalent radii of distribution ellipses, the solution of the problem presents a great inconvenience and is very slow in time.

In this research, let us consider a possible increase in the number of equations for solving the system by using differentials in estimating the equivalent radii of the ellipses of the peak distribution of the Raman polarization spectrum when gold nanoparticles are identified on the surface of polyester fibers.

It is not possible to provide a solution to a system of nonlinear quadratic equations with a number of parameters up to 9 in the ordinary analytic algebraic form because of the unwieldiness of the record. In this research, the authors used the method of compiling only quadratic differential correlation equations with two unknowns for solving a vector-matrix problem for the possibility of moving to a system of equations with a large number of unknowns.
2. Materials and methods
Experiments on the measurement of random values were preliminarily carried out, the spectra of the PE fibers were obtained (Picture 1), and correlation matrices and distribution parameters (1) were found (out) taking into account the polarization of the radiation in X and Y directions.

Analysis of the data obtained showed that the correlation matrices have a wide range of values ranging from 0.994549 to 0.420535 without gold nanoparticles, and for fibers with nanoparticles the range (is) from 0.934366 to -0.242178. This indicates that gold nanoparticles decrease the correlation.

![Figure 1. Spectrograms of Raman scattering: a - polarization across PE fibers with gold nanoparticles; b - polarization along the PE fibers with gold nanoparticles](image)

The distribution parameters (1), in particular, the mathematical expectations differ significantly in the intensity of the spectral peaks with polarization across fibers X and along the Y fibers. A key feature is that the mean intensities for polarization along the fibers are the intensity of central peaks 4, 5, 6 and 7 is much higher than extreme peaks 1, 2, 3, 8 and 9 almost 20 times. The central peaks in X have practically the same intensity with extreme peaks, and some extreme peaks are even larger than the central one for fibers without nanoparticles. This indicates that the maximum efficiency of measurements of Raman spectra during polarization along the fibers has been revealed. However, the problem arises of checking the information saturation when measuring the peaks of the Raman spectra of Raman radiation.

\[
\begin{align*}
\text{MEN}_X & = (416.914 \ 152.378 \ 227.443 \ 400.725 \ 398.847 \ 502.157 \ 514.102 \ 278.196 \ 499.456) \\
\text{MEN}_Y & = (525.478 \ 321.605 \ 854.972 \ 3861.032 \ 2872.996 \ 1258.934 \ 1268.02 \ 143.918 \ 151.002) \\
\sigma & = (70.798 \ 27.978 \ 41.622 \ 53.385 \ 41.117 \ 72.298 \ 67.912 \ 35.079 \ 56.89) \\
\sigma & = (50.752 \ 29.74 \ 79.231 \ 259.348 \ 270.86 \ 100.309 \ 113.697 \ 6.59 \ 14.109) \\
\text{MEN}_X^0 & = (745.336 \ 307.767 \ 387.809 \ 3861.032 \ 2872.996 \ 1258.934 \ 1268.02 \ 143.918 \ 151.002) \\
\text{MEN}_Y^0 & = (972.254 \ 606.828 \ 1598.202 \ 5178.102 \ 5128.382 \ 2304.268 \ 2288.106 \ 238.792 \ 234.17) \\
\sigma & = (196.404 \ 93.691 \ 81.964 \ 121.371 \ 166.386 \ 186.764 \ 241.501 \ 89.597 \ 175.22) \\
\sigma & = (221.83 \ 133.433 \ 358.411 \ 1038.421 \ 1030.864 \ 473.166 \ 455.166 \ 35.978 \ 32.436)
\end{align*}
\]  

(1)

During the solution of the system of differential correlation equations, an uncertainty was revealed that when checking a solution for the graphical intersection of distribution ellipses without nanoparticles and with gold nanoparticles, two intersection points appeared. In this case, the equivalent radius of the ellipses was not equal to the radius that was found out during the solution.
However, the accuracy of the intersection of the distribution ellipses depends on the choice of additive $\Delta$. The curvature radii for the point of intersection of the ellipses of the intensity distribution of the reradiation spectra of the Raman spectra (4-5) are found out from the coordinates of ellipses $v_0$ and $v_1$:

$$v_0 = -2.77 \times 10^{-2} \quad \text{and} \quad v_1 = 8.88 \times 10^{-16}$$

The accuracy of the solution of the system of equations is high: $f(v_0, v_1) = 8.88 \times 10^{-16}$. This accuracy can be used for preliminary results.

To compose a system of differential correlation equations, $R$ is (used) - the radius of curvature of the intersection of distribution ellipses in vector-matrix analytic expressions along the coordinates of the points of intersection. In this research let us consider a system of only two vector-matrix analytic expressions $R^2 = X^{-1} \Sigma^{-1} X$ for $R_0$ and $R_1$.

The analytical expression for differential correlation equation $g(x, y)$ is obtained by differentiating equation $f(x, y)$ with respect to $X$. It is necessary to choose addition $\Delta$.

To formulate a system of differential correlation equations, $R$ is (used) - the radius of curvature of the intersection of distribution ellipses in vector-matrix analytic expressions along the coordinates of the points of intersection. In this research let us consider a system of only two vector-matrix analytic expressions $R^2 = X^{-1} \Sigma^{-1} X$ for $R_0$ and $R_1$.

The accuracy of the solution of the system of equations is high: $f(v_0, v_1) = 8.88 \times 10^{-16}$ and $g(v_0, v_1) = -2.77 \times 10^{-17}$ (4). It shows a divergence in the accuracy of equivalent radii $R_0$ and $R_1$ to $10^{-16}$. However, the accuracy of the intersection of the distribution ellipses depends on the choice of additive $\Delta$.

\[ \sum 0 = \begin{pmatrix} 1 & r_{X_0i,j} \\ r_{X_0i,j} & 1 \end{pmatrix}, \quad \sum 0 = \begin{pmatrix} 1 & r_{X_1i,j} \\ r_{X_1i,j} & 1 \end{pmatrix} \] (2)

\[ g(x,y) = \frac{dx}{dx} \begin{pmatrix} x - MENX_x \\ y - MELY_y \end{pmatrix} \sum \left[ \begin{pmatrix} x - MENX_x \\ y - MELY_y \end{pmatrix} \frac{\delta X}{\delta Y_j} \right] - \frac{dx}{dx} \begin{pmatrix} x - MENX_0x \\ y - MELY_0y \end{pmatrix} \sum \left[ \begin{pmatrix} x - MENX_0x \\ y - MELY_0y \end{pmatrix} \frac{\delta X_0}{\delta Y_0j} \right] + 0.02985 \] (3)

\[ f(x,y) = \begin{pmatrix} x - MENX_0x \\ y - MELY_0y \end{pmatrix} \sum \left[ \begin{pmatrix} x - MENX_0x \\ y - MELY_0y \end{pmatrix} \frac{\delta X_0}{\delta Y_0j} \right] - \frac{dx}{dx} \begin{pmatrix} x - MENX_x \\ y - MELY_y \end{pmatrix} \sum \left[ \begin{pmatrix} x - MENX_x \\ y - MELY_y \end{pmatrix} \frac{\delta X}{\delta Y_j} \right] \] (3)

$x := 400.0 \quad y := 1590.0$

Given

\[ f(x,y) = 0 \]
\[ g(x,y) = 0 \]
\[ v := \text{Find}(x,y) \]

\[ v = \begin{pmatrix} 412.301842 \\ 1469.164736 \end{pmatrix} \]

\[ g(v_0,v_1) = -2.7755575615628914 \times 10^{-17} \]

\[ f(v_0,v_1) = 8.8811784197001252 \times 10^{-16} \]

3. Results and Discussion

The curvature radii for the point of intersection of the ellipses of the intensity distribution of the reradiation spectra of the Raman spectra (4-5) are found out from the coordinates of ellipses $v$ ($v_0$, $v_1$):

\[ v = \text{Find}(x,y) \]

\[ v = \begin{pmatrix} 412.301842 \\ 1469.164736 \end{pmatrix} \]
\[
R_{0,i,j} = \sqrt{\left( \frac{\delta_0 - \delta X_{0,i}}{\sigma \Delta X_{0,i}} \right) \cdot \left( \frac{\delta_1 - \delta Y_{0,i}}{\sigma \Delta Y_{0,i}} \right)} \cdot \left( \sum \right)^{-1} \cdot \left( \frac{\delta_0 - \delta X_{1,i}}{\sigma \Delta X_{1,i}} \right) \cdot \left( \frac{\delta_1 - \delta Y_{1,i}}{\sigma \Delta Y_{1,i}} \right)
\] (4)

\[
R_{1,i,j} = \sqrt{\left( \frac{\delta_0 - \delta X_{1,i}}{\sigma \Delta X_{1,i}} \right) \cdot \left( \frac{\delta_1 - \delta Y_{1,i}}{\sigma \Delta Y_{1,i}} \right)} \cdot \left( \sum \right)^{-1} \cdot \left( \frac{\delta_0 - \delta X_{0,i}}{\sigma \Delta X_{0,i}} \right) \cdot \left( \frac{\delta_1 - \delta Y_{0,i}}{\sigma \Delta Y_{0,i}} \right)
\] (5)

\[R_0 = 1.8395181499853053\]
\[R_1 = 1.8395181499853055\]

If the additive will not be \(\Delta = +0.02985\) and if \(\Delta = 0.0000\), the equivalent radius will be:
\[R_0 = 1.8828855390789887\] and \[R_1 = 1.8828855390789887\]

**Figure 2.** Graphical estimation of the intersection of the ellipses of the distribution of Raman spectra in the identification of nanoparticles in the polarization of Y-along and X-across the fibers at \(\Delta = +0.02985\); a - a general view; b - enlarged fragment of points of intersection.
Figure 3. Graphical evaluation of the intersection of the ellipses of the distribution of Raman spectra in the identification of nanoparticles in the polarization of Y-along and X-across the fibers at \( \Delta = 0.000 \): a - a general view; b - enlarged fragment of points of intersection

It should be noted that when solving differential equations (1-2), (the) uncertainty was revealed in the results, since ellipses intersection occurs at two points (picture 2) due to the increased radius distribution ellipses Raman spectra polyester without nanoparticles and gold nanoparticles.

Then it becomes necessary to introduce additive \( \Delta = + 0.02985 \). In this case, the ellipses intersect at one point (Picture 1) and the uncertainty disappears. However, this value of the additive is applied only for one particular solution of the system of equations for certain parameters. For other parameters, the value of the additive must be selected manually. It makes it difficult to obtain results with high accuracy and with high speed. For 2.2% accuracy, the solution can be carried out without adding (\( \Delta = 0.000 \)) for any parameters of the system of differential equations and used for preliminary results.

4. Conclusion

The practical accuracy of obtaining the results depends on the necessary resolving power (sensitivity) of the proposed method for identifying gold nanoparticles. In order to ensure resolution of 1-2% concentration of gold nanoparticles that are on the fibers, it is necessary to carry out processing results with precision (1-2) \( \times 10^{-4} \), and the accuracy of the values of each parameter (1-2) \( \times 10^{-6} \).

In this paper, the accuracy of the solution is determined by equation \( f (v_0, v_1) = 8.88 \times 10^{-16} \) and by equation \( g (v_0, v_1) = -2.77 \times 10^{-17} \). Accuracy of obtaining parameters \( R_0 \) and \( R_1 \) is up to \( 10^{-16} \). The accuracy of calculating the uncertainty at the intersection of ellipses is 2.2% for equations without the addition of \( \Delta \), and depending on the accuracy of addition \( \Delta \), the accuracy of calculating coordinates for solving the equations with the addition of \( \Delta \) also depends.

The task of further research is as follows: to carry out research on the solutions of a system of differential equations when differentiating along X and Y, to combine these methods in differentiating with respect to X and Y, simultaneously, to exclude the use of the additive.
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