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QUALITY ESTIMATION THE OF MAXIMUM-LIKELIHOOD ALGORITHM TO THE TASK OF SPACE DISTRIBUTION OF ELEMENTS BY PIXE

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The numerical research is carried out for different approximations of likelihood-function and Fisher's matrix with reference to maximum-likelihood algorithm at determination of impurity profile of certain chemical element in researched sample by PIXE. It is shown, that the testing of this algorithm, previously led, points to a basic opportunity of its application for restoration of impurity profile by PIXE. However, its practical application causes difficulties, and the expression offered earlier for likelihood-function does not allow determining accuracy of restoration of impurity profile. The problems preventing from opportunity of practical use of algorithm are studied.

INTRODUCTION

PIXE (proton induced x-ray emission) method is widely used for analysis of element composition of materials, it possess good metrological characteristics and allows to investigate space distribution of elements. At the basis of such measurements there is X-ray registration under different angles to the sample surface, measurement of lines intensity ratio in multyplete (K_α/K_β), measurement of X-ray radiation yield for different energy of incident particles. Mathematically, this procedure is described by integral equation of the first kind which will be considered further. Experimental scheme as well as algorithm of profile reconstruction (iterative maximum-likelihood algorithm) of impurity in case of energy variation of incident radiation is given in the work [1]. Besides, additional aspects of this algorithm application are considered in the work of authors [2].

The maximum-likelihood algorithm for impurity profile reconstruction in the investigated sample by means of characteristic X-Ray radiation is given in the work [1]. However, its sufficient mathematical basis is not given. This algorithm refers to mathematical statistics. Analysis of accuracy of results reconstruction from the point of view of this region of mathematics is not given in [1]. Only results of computational simulation which should be recognized as satisfactory are given in this work. We have carried out a detailed testing of the offered algorithm, results of which are given in [2]. At that, there have been discovered circumstances which were not mentioned in the work [1], and we do not know whether its authors faced this. The authors [1] did not give the basis of that type of likelihood function which follows from its exact expression. According to our opinion, in the work [1], in the expression which is used for probability function, one item is emitted. Therefore, the algorithm is built on the basis of truncated type of likelihood function.

The algorithm of profile reconstruction by means of the maximum-likelihood method is iteration. At that, each new approximation should be more close to exact solution than the previous one. During testing, we have faced with the fact that iteration process does not coincide with initially given test profile. This appears in the following. In the algorithm the parameter is used: absolute error of the algorithm $\Delta_{\alpha lg}$. It is a module of maximal deviation between two approximations obtained on successive iterations. At iteration process, this value reduces, and it was expected that obtained approximations will be tending to test variant. However, it turned out that this condition is not fulfilling. At the beginning, the obtained approximations are quasi to test profile, at some algorithm error they turn out to be close to it, but then increase of discrepancy is observed. At introduction of yield error of X-ray radiation, minimal deviation of computation and test variant was increasing with increase of modeling error of X-ray radiation.

Thus, question of stop criteria of algorithm work appeared. It was not still clear weather the likelihood function reaches maximal meaning? What approximation is more close to real one? During the process of numerical simulation we have determined that maximum-likelihood algorithm, theoretically, allows to obtain solution with satisfactory quality of test profile restore. However, without a substantiated answer to the question of adequacy of the reconstructed profile to a real one, the practical use of algorithm turns out to be impossible. In the work [1] these questions are not considered. Their solution can be reached by using a mathematical statistics. To do this, it is necessary, from the given in [1] simplified expression for logarithm of probability function, to obtain its approximation which, on the one hand, is suitable for practical use, and, on the other hand, would reflect the investigated process with maximal reliability.

To determine quality estimations of profile reconstruction it is necessary to obtain, first of all, Fisher matrix. It is a set of negative secondary derivatives from logarithm of probability function per its arguments. In the point of maximal probability the Fisher matrix should be positively determined. The matrix, inverse to Fisher matrix, - is a covariance matrix, which contains information about error of the reconstructed profile.

Square roots from its diagonal elements give estimation to standard deviation of the obtained solution. In more details these questions will be considered below.

In the present work, some approximations for logarithm of likelihood function which could be obtained from results given in the work [1] are investigated. Besides, performance of covariance matrix and Fisher matrix corresponding to these approximations, and possibility of their application to obtain quality estimations of profiles reconstruction are investigated. To solve set tasks the same three profiles are used: Gaussian, monotone increasing and monotone decreasing which had been considered in [1, 2].

1. MAXIMUM LIKELIHOOD ALGORITHM

The experimental scheme to determine impurities concentration in the investigated sample according to characteristic X-Ray radiation is given in [1, 2] in more details. But the concentration itself can be obtained by solving an integral equation which looks like:

$$Y(E_0,\theta,\varphi)=\frac{\eta N_p \Omega}{4\pi}\int_0^{R\cos\theta} c(x)\sigma(E(x))\exp(-\mu x/\cos\varphi)dx\,, \qquad (1)$$

where $Y(E_0,\theta,\varphi)$ is experimentally measured yield of X-Ray radiation; θ – angle between normal to surface of the investigated sample and incident protons beam; φ – angle between normal to surface of the sample and direction of registration of characteristic X-Ray radiation; N_p – quantity of protons which have fallen on the target; η – proper detector efficiency with respect to the registered quanta; Ω – detector solid angle; $c(x)$ – impurity concentration as a depth function x; $\sigma(E(x))$ – cross-section of excitation of characteristic X-Ray radiation by protons with energy$E$; μ – factor of absorbing of X-Ray radiation in the investigated sample; R– protons track range with maximal energy in the investigated sample. In [2] it is noted that equation (1) is an integral equation of the first type, and the task of its solution is incorrect. Mathematical side of this question is shortly given in [2], and also in the literature which is quoted there. Discretization of equation (1) leads to the following set of linear algebraic equations:

$$Y_i = \sum_j A_{ij} c_j\,, \qquad (2)$$

where

$$Y_i=Y(E_{0i},\theta,\varphi)\,,\ A_{ij}=\frac{\eta N_p \Omega}{4\pi}\int_{x_{j-1}}^{x_j}\sigma(E(x))\exp(-\mu x/\cos\varphi)dx\,.$$

Matrix elements A_{ij} are determined by experimental conditions and composition of the investigated sample. At small impurity concentration, its influence on bremsstrahlung loss of protons and absorption of X-Ray radiation in the sample can be neglected. In this case, integral equation (2) is a linear one, and matrix elements A_{ij} do not depend upon c_j. In many cases, due to matrix A_{ij} is ill-conditioned, the solution of the system (2) by conventional methods leads to oscillations and instability.

To overcome these difficulties, various methods of regularization are used. Some of them are given in works [3-7]. Experimental data Y_i at practice are known with some error and have random character. Theoretically, the system (2) should be replaced by the following:

$$Y_i = \sum_j A_{ij} c_j + \varsigma_0 \qquad (2a)$$

where ς_0 – random background, specific realization of which is not known. In general case, matrix elements $A_{ij\,\mathrm{j}}$ are also random. Substantively, specific meanings of the value c_j are deterministic but as a result of randomness Y_i those values C_j which are under determination from the set of equations (2), we are forced to consider them as random. Thus, to solve (2) statistical methods could be used. Such a method is a maximum-likelihood method which is used in [1,2], is given in details, for instance, in [8,9]. In its basis is use of likelihood function which depends upon c_j concentration as well as experimental data Y_i. Statistical property of Y_i are described by conditional density of probability f(Y|c) for experimental data Y at c concrete realization. But this density of probability can be considered as a function from c at Y meanings which have been specifically obtained in the experiment. In this case it named likelihood function. The sense of algorithm is: set of c_j values at which function of probability has maximum is searched for.

In [1], algorithm of construction of likelihood function for the considered task is offered. Y_i detecting value is an overall quantity of X-Ray quanta which have come on the counter and can be shown as:

$$Y_i = \sum_j X_{ij}\,, \qquad (3)$$

where X_{ij} is a flux of X-Ray radiation from j-slice of the sample which is situated between depths x_{j-1} and x_j for energy meaning of the incident proton beam equal to E_i. The values X_{ij} are random Poisson and have density of probability;

$$h_{ij}(X_{ij},c_j)=\exp(-A_{ij}c_j)\frac{(-A_{ij}c_j)^{X_{ij}}}{X_{ij}!}\,. \qquad (4)$$

$A_{ij}c_j$ is an average meaning of X_{ij}. Density of probability for the whole set of X_{ij} is equal to $h(X,c)\equiv h(X\mid c)$. Density of probability $h(X,c)\equiv h(X\mid c)$ is a function from X at given c meanings upon which it depends as from parameter. If to consider it as a function from c then we obtain the likelihood function. The task is to determine such set $c=\{c_j\}$ for given Y_i at which the likelihood function is maximal. For practical purposes, logarithm of probability function is usually used:

$$\ln h(X,c)=\sum_i\sum_j\left[-A_{ij}c_j + X_{ij}\ln(A_{ij}c_j)-\ln(X_{ij}!)\right]. \qquad (5)$$

X_{ij} values are not directly registered, they are connected with Y_i correlation (3). Maximal likelihood solution for matrix equation (2) can be obtained as set of such c_j at which the conditional density of probability (or its logarithm) has maximum at condition (3). The task of determination of maximum of conditional density of probability at fulfilling (3) and current meanings $c_j^{(m)}$ (which correspond to m -th iteration and are used to find the following approximation $c_j^{(m+1)}$) can be solved by iteration method. In [1], without obtaining, it is offered an expression for X_{ij} at given Y_i and current meanings of $c_j^{(n)}$ which looks like the following:

$$M_{ij} = X_{ij}^{(m)} = \frac{A_{ij}c_j^{(m)}}{\sum_p A_{ip}c_p^{(m)}} Y_i. \quad (6)$$

And for logarithm of conditional density of probability the expression is used:

$$\ln h^{(m+1)}(X, c \mid Y, c^{(m)}) = \sum_i \sum_j \left[-A_{ij}c_j + M_{ij} \ln(A_{ij}c_j) \right] - V, \quad (7)$$

where $V = \sum_{i,j} \ln(X_{ij}!)$. New approximation for c_j is obtained by maximization of likelihood function (7) for which its partial derivatives with respect to c_j are equal to zero:

$$\frac{\partial}{\partial c_j} \ln h^{(n+1)} = \sum_i \left(-A_{ij} + \frac{M_{ij}}{c_j} \right) = 0 \quad (8)$$

whence it is evident:

$$c_j^{(m+1)} = \frac{\sum_i M_{ij}}{\sum_i A_{ij}}. \quad (9)$$

As initial approximation it is taken constant which is equal to meaning averaged according to all results of measurements:

$$c_j^{(0)} = \frac{1}{n} \sum_{i=1}^{n} \left(Y_i / \sum_k^n A_{ik} \right), \quad (10)$$

where n is a number of measured yields of X-Ray radiation.

As it is clear from (7)-(9), addendum $V = \ln(X_{ij}!)$ in algorithm of approximated type of likelihood function is not used. Besides, likelihood function depends from previous approximation. Such an approach in the work [1] is not substantiated. Instrument of mathematical statistics allows to make estimation of standard deviation for the found optimal meanings of c_j. To do this, first of all, it is necessary to determine informational Fisher matrix (see, for instance, [8, 9]) which must be positively determined and looks like:

$$I_{k,l}(c) = \left\langle -\frac{\partial^2}{\partial c_k \partial c_l} \ln h \right\rangle, \quad (11)$$

where angle brackets mean averaging along all Y realizations. Matrix which is inverse to Fisher matrix ($C = I^{-1}$) is called a covariance matrix. Square roots from its diagonal elements determine-mean-square deviation of the found c_j values. As it is clear from the given type of likelihood function (5)-(7), the yield of X-Ray radiation is a random value (Y_i) which is to be determined experimentally, i.e., addendum ς_0 in equation (2a) is equal to zero – this is not taken into account. So, further, at computation of Fisher matrix averaging is not carried out. Account of random background in equation (2a) with reference to the given task requires separate consideration. In literature on mathematical statistics (see, for example [8,9]) is usually considered the very mathematical formulation for the task (2)-(2a) in which it is presupposed that approximately given only the right part of the set of linear algebraic equations which has Gaussian scattering, whereas matrix elements are known precisely. In the task which we are considering, values $A_{ij}c_j$ are presupposed as random.

2. ANALYSIS OF POSSIBLE VARIANTS OF LIKELIHOOD FUNCTION

Approximation of likelihood function which is used in [1] and determined by expression (7) depends upon current meanings of c_j as well as previous approximation $c_j^{(m)}$, however, such approach is not coordinated with the one which is accepted in mathematical statistics. Since its substantiation in the article [1] is not given, then to solve the problems given in introduction, we modify expression (7) for likelihood function by using the results given in [1]. First of all, express likelihood function only through current meanings of c_j. To do this, consider that M_{ij} which is determined by formula (6) depends upon current c_j, and V which is a part of (7) and is not used in algorithm of probability, present like this:

$$V = \ln(M_{ij}!). \quad (12)$$

Then, expression for likelihood function will look like this:

$$\ln h(Y \mid c) = \sum_i \sum_j \left[-A_{ij}c_j + M_{ij} \ln(A_{ij}c_j) - \ln(M_{ij}!) \right] \quad (13)$$

and for M_{ij}

$$M_{ij} = \frac{A_{ij}c_j}{\sum_p A_{ip}c_p} Y_i. \quad (14)$$

Then, in formula (13) it is necessary to transform expression $\ln(M_{ij}!)$. To do this, we use generalization

of factorial in case of continuous quantities: $M_{ij}! = \Gamma(M_{ij}+1)$, where $\Gamma(x)$ is gamma-function, and for transformation of $\ln\left[\Gamma(M_{ij}+1)\right]$ we will use asymptotic series of Stirling [10]:

$$\ln(x!) = \ln\left[\Gamma(x+1)\right] = \frac{1}{2}\ln(2\pi) - x + \left(x+\frac{1}{2}\right)\ln x + \quad (15)$$
$$+\frac{B_1}{2x} - \frac{B_2}{12x^3} + \frac{B_3}{30x^5} - \ldots$$

where $B_1 = 1/6,\ B_2 = 1/30,\ B_3 = 1/42\ldots$. – numbers of Bernully. Absolute error of series is less than the first rejected member. This series is not a convergent one. Its application is problematic at $x < 1$, i.e., $X_{ij} \square 1$ or $X_{ij} < 1$. Such a situation is possible in the field of large depths or very small concentrations of impurities when X-Ray radiation can be unregistered.

Expressions (13) – (15) are used for analytical computation of informational Fisher matrix (11) which, due to its lengthiness, is not given here. Theoretically, it can be found by means of using computation differentiation. However, such a procedure itself is incorrect and unstable (similarly to solution of integral equation (1)). In case of large number of variables for computation of secondary derivatives, it is necessary to use differential formulas of high preciseness. But in this case, the task of averaging in the formula (11) which is to be carried out numerically complicates essentially, and this can require unacceptably huge costs of calculation time.

Thus, the final goal of our research is computation of covariance matrix and determination of root-mean-square error for profile reconstruction. As it is clear from the mentioned above, various variants of likelihood function which are determined by number of addendum that contain factors B_i in asymptotic series of Stirling can be offered. Let's note, that algorithm which is determined by formula (9) is used for profiles reconstruction. It is not connected with those variants of likelihood function which are determined by expressions (13), (14) and (15). The results given below are needed to be considered as preliminary researches. They allow to determine the ways of solution of problems which are mentioned in the introduction. Investigation of likelihood function and covariance matrix has been carried out by means of numerical simulation using three profiles of distribution of phosphorus impurities in silicon sample which have been considered in [2], Gaussian, monotone increasing and monotone decreasing. Use of algorithm (9) can be justified in this case by the fact that at different variants of likelihood function it was increasing.

Our task is (to):

a) to obtain type of likelihood function which is mathematically substantiated, approximated, suitable for practical use but adequate to experimental conditions;

b) informational Fisher matrix, which was generated by it, should be positively determined;

c) make sure on test tasks that error estimation of reconstructed profiles which was obtained by covariance matrix decreases with decrease of error of yield of X-Ray radiation.

The last item is a criterion of practical applicability of algorithm. At that, such an conclusion can be made according to results of considerable volume of numerical simulation and processing of experimental results with previously known distribution of impurity profile. Information weather such investigations have been carried out by the authors of the work [1] is not available for us. Motives of formulating the very tasks come from results of preliminary numerical simulation.

3. NUMERICAL INVESTIGATION OF VARIOUS VARIANTS OF LIKELIHOOD FUNCTION

3.1. GENERAL ISSUES OF COMPUTATIONAL MODELING

At numerical simulation of likelihood function, as it was mentioned before, three test profiles were used as well as in the work [2]. At that, it was checked weather Fisher matrix and covariance matrix are positively determined. Positive determines of Fisher matrix was determined by computation of its eigenvalues which, in this case, should be positive. Type of likelihod function was changed by equalization to zero of factors $B_i,\ i = 1,\ 2,\ 3$ in expression (15). At that, the corresponding addendum were rejected. At the beginning, all three factors were equal to zero, and then in series to each of them the initial meaning was given back. During the process of numerical simulation, deviations of the right part which was reconstructed by current m-th approximation $c_j^{(m)}$ was controlled

$$Y_i^{(m)} = \sum_j A_{ij} c_j^{(m)} \quad (16)$$

from given Y_i. To do this, three types of error were used: maximal absolute error $\Delta_{abs} = \max_i \left|Y_i - Y_i^{(m)}\right|$, maximal relative error $\Delta_r = \max_i \left(\left|Y_i - Y_i^{(m)}\right| / Y_i\right)$, and also summarized absolute error $\Delta_\Sigma = \sum_i \left|Y_i - Y_i^{(m)}\right|$. The profile reconstruction was usually beginning from the meaning of absolute error of algorithm $\left(\delta_{\text{alg}} = \max_j \left|c_j^{(n)} - c_j^{(n+1)}\right|\right)$ which made (0.1 – 1)% from average density of impurity and was decreasing in 2 or 2.5 times, and in each decade of orders 10^l was taken in correspondence to series (5, 2, 1). Concentration of c_j was, in fact, density which was expressed in atomic units (number of atoms in sm^3). With sample density $10^{22}\ldots 110^{23}$ sm^{-3}, characteristic values of c_j have order $10^{20}\ldots 10^{21}$ at concentration of impurity in several atomic percentage. For all investigated profiles, with decrease of Δ_{alg} the decrease of all mentioned three types of error was happening.

3.2. INFLUENCE OF THE WAY OF CALCULATION OF THE RIGHT PART OF THE TASK ON RESULTS OF PROFILE RECONSTRUCTION

In introduction it was mentioned that while testing of (see [2]) maximum-likelihood algorithm for all three types of profile, there is optimal value of algorithm error $\Delta_{a\lg}$ at which the reconstructed profile was mostly close to the testing one, could have been mentioned. At further decrease of this parameter the calculated approximation was beginning to deviate from the test profile. The reason for this lies in the following circumstance. Likelihood function (5) and numerical algorithm (9) have been obtained not for initial integral equation (1) but for matrix equation (2) (for the set of linear algebraic equations). In the work [2] the right part of matrix equation (2) have been computed without connection with elements of matrix A_{ij}, but by means of thorough calculation of integral in the left part (1) by the method of trapezium with preciseness up to 5-6 decimal digits. However, such data for matrix equation (2) are less precise. "Correct" are only those Y_i values, which are obtained at substitution in the left part (2) of test c_j values. We have checked this variant for all three profiles. Fig. 1 shows the reconstructed Gaussian profile which is the closest to the test one, for yield of X-Ray radiation computed by numerical integration.

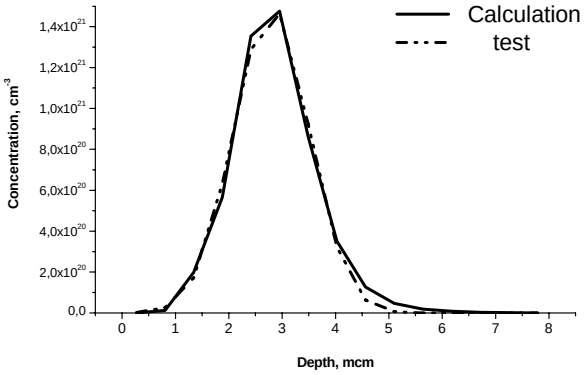

Fig. 1. Algorithm error $5.0\cdot10^{16}$. The reconstructed Gaussian profile which is the closest to the test one. Y_i has been computed by formula (1)

With decrease of absolute error of algorithm $\Delta_{a\lg}$, the reconstructed profile begins to deviate from the test one in maximum region and for depths more than 3 mkm. It is shown at fig. 2. Fig. 3 and 4 show the result of reconstruction of Gaussian profile in case when computation of yield of X-Ray radiation Y_i, for identical values of c_j is carried out by formula (2). Values of parameter $\Delta_{a\lg}$, at fig. 3 and 4 are identical to those, which are used for profiles that are shown at fig. 1 and 2 correspondingly.

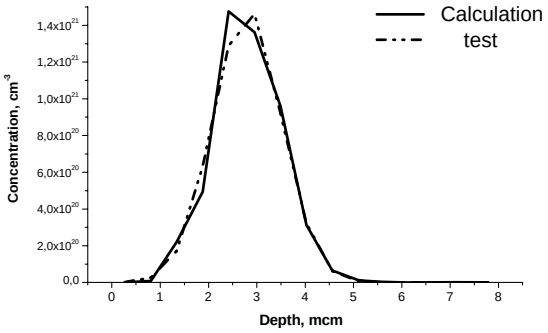

Fig. 2. Algorithm error $5.0\cdot10^{15}$. Decrease of $\Delta_{a\lg}$, parameter leads to deformation of the reconstructed profile relatively to the test one. Y_i has been computed by formula (1)

As it is clear from fig. 3-5, with precise enough initial data of the task, the of maximum-likelihood method allows to find solution of the given task reliably and without deformations. If Y_i is computed by formula (1) and to use matrix equation (2) for the profile reconstruction, then, at condition of $\Delta_{a\lg} < (2\ldots5)\cdot10^{16}$, the reconstructed profile is distorted essentially. Similar results have been obtained for other test profiles also.

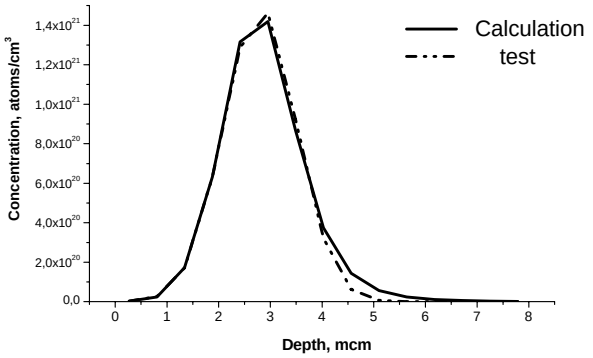

Fig. 3. Algorithm error $5.0\cdot10^{16}$. Gaussian profile which has been reconstructed for data of Y_i computed by formula (2)

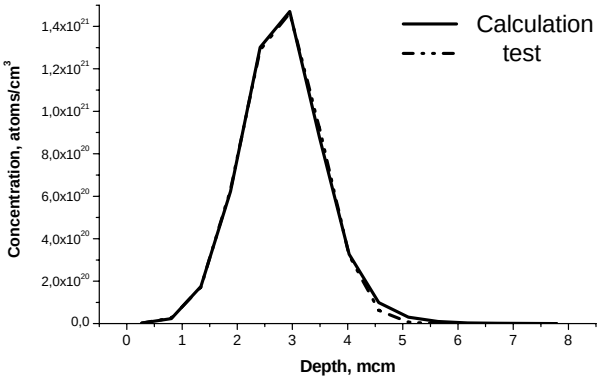

Fig. 4. Algorithm error $5.0\cdot10^{15}$. The profile has been computed according to data which are identical to fig. 3, but with other meanings of $\Delta_{a\lg}$

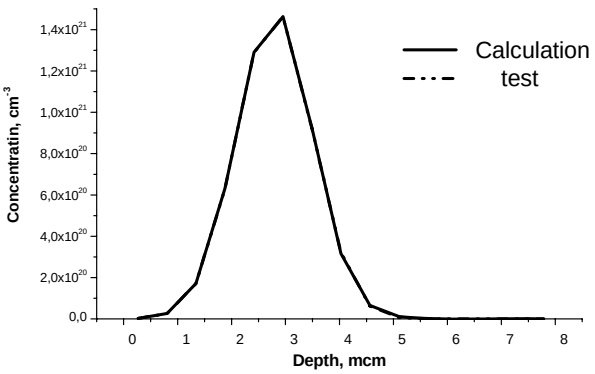

Fig. 5. Algorithm error $5.0 \cdot 10^{12}$. The profile which has been reconstructed according to data that has been computed by formula (2) but with other meaning of $\Delta_{a\lg}$ which is more (essentially) less than at fig. 3, 4

The results of Y_i computation which has been obtained by both ways for Gaussian profile, are shown in the table 1.

Table 1

Yield of X-Ray radiation for test tasks which have been computed by two ways

#	Energy, MeV	Yield of X-Ray radiation of Y_i which has been computed by formula (1) by means of integratio	Yield of X-Ray radiation of Y_i which has been computed by formula (2) using A_{ij} matrix
1	0.6	$8.223 \cdot 10^2$	$1.721 \cdot 10^3$
2	0.7	$3.646 \cdot 10^3$	$5.281 \cdot 10^3$
3	0.8	$1.180 \cdot 10^4$	$1.314 \cdot 10^4$
4	0.9	$3.010 \cdot 10^4$	$3.326 \cdot 10^4$
5	1.0	$6.637 \cdot 10^4$	$7.074 \cdot 10^4$
6	1.1	$1.268 \cdot 10^5$	$1.320 \cdot 10^5$
7	1.2	$2.101 \cdot 10^5$	$2.160 \cdot 10^5$
8	1.3	$3.0856 \cdot 10^5$	$3.148 \cdot 10^5$
9	1.4	$4.121 \cdot 10^5$	$4.186 \cdot 10^5$
10	1.5	$5.132 \cdot 10^5$	$5.200 \cdot 10^5$
11	1.6	$6.078 \cdot 10^5$	$6.149 \cdot 10^5$
12	1.7	$6.945 \cdot 10^5$	$7.019 \cdot 10^5$
13	1.8	$7.735 \cdot 10^5$	$7.812 \cdot 10^5$
14	1.0	$8.459 \cdot 10^5$	$8.540 \cdot 10^5$
15	2.0	$9.127 \cdot 10^5$	$9.211 \cdot 10^5$

As it is clear from this table, there are differences in yield of X-Ray radiation which has been computed by two ways, they are the most essential in small energies of probing beam.

During the process of numerical simulation, deviations of the restored values $Y_i^{(m)}$ (16) from given Y_i were controlled. For values Y_i which have been computed by expression (1) the maximal relative error Δ_r at which the reconstructed profile was the closest to the test one made 0.00004 for monotone decreasing profile, 0.0026 for monotone increasing one, 0.04 for Gaussian one. Further, with increase of deviation of the reconstructed profile from test one, this error was decreased. Such regularity was observed for Δ_{abs} and Δ_Σ. For initial data which has been computed by formula (2) Δ_r made $10^{-5}\ldots10^{-6}$ at minimal values of $\Delta_{a\lg}$ which were used in this case.

3.3. CHARACTER OF PERFORMANCES OF LIKELIHOOD FUNCTION, FISHER MATRIX AND COVARIANCE MATRIX AT ITERATION PROCESS

With respect to the mentioned results, the question about character of behavior of likelihood function in iteration process appears. Let's pay attention to the circumstance that algorithm (9) directly is not related to the investigated variants of likelihood function (13)-(15), and the task of this stage of investigation is, first of all, in obtaining of preliminary results on the problem we are interested in. Practically for all studied profiles and for both ways of computation of the right part during iteration process the increase of likelihood function in the all used range of parameters has been observed. The exception was only increasing profile with initial data Y_i which has been obtained by formula (2). In this case, with values $\Delta_{a\lg}$ from $2.0 \cdot 10^{15}$ and less, gradual decrease of likelihood function has been observed. Such behavior was typical for all types of likelihood function (13)-(15). For all profiles with the sequence account of B_1 factors in expression (15) difference between its corresponding values has been decreasing and for variants ($B_1 \neq 0$, $B_2 \neq 0$, $B_3 \neq 0$) and ($B_1 \neq 0$, $B_2 \neq 0$, $B_3 \neq 0$) difference has been observed in 5th and 6th decimal digit. It is followed from the mentioned above that despite numerical algorithm (9) does not go directly from the used variants of probability function (13)-(15), nevertheless, it leads to its maximization.

The other side of the problem we are interested in is to obtain covariance matrix which gives root-mean-square estimation of error of the reconstructed profile. Covariance matrix and Fisher matrix have been considered for all three previously mentioned profiles, for different variants of likelihood function and for two types of initial data Y_i which has been computed by formulas (1) and (2). For Fisher matrix (11), analytical expression has been obtained and it corresponds to all variants of likelihood function, and which, due to its inconvenience, is not given here. Fisher matrix by the sense of its definition should be positively determined. Covariance matrix has been obtained by numerical inverse of Fisher matrix. All diagonal elements of the last should obligatory be positive because likelihood function should have maximum. To find out, whether Fisher matrix is positively determined, its eigenvalues have been numerically determined, which, in this case, should be positive.

In most cases which are given here, Fisher matrix had negative eigenvalues and its positive determines was rather an exception than a rule. The lowest number of negative eigenvalues of matrix was in the case when

all three B_1 factors were not equal to zero. In a number of cases, when Fisher matrix was positively determined, covariance matrix could not have been computed due to ill-condition of matrix (11). In table 2 there are results of error computation for monotone increasing profile initial data for which have been modeled by formula (2).

Table 2

Reconstructed monotonically increasing profile for Y_i, calculated by formulae (2) with mean-square error

#	Depth, mkm	Test values, cm^{-3}	Reconstructed values, cm^{-3}	Standard error, cm^{-3}
1	0.268	$1.370 \cdot 10^{20}$	$1.371 \cdot 10^{20}$	$0.118 \cdot 10^{20}$
2	0.805	$3.747 \cdot 10^{20}$	$3.744 \cdot 10^{20}$	$0.523 \cdot 1\text{-}^{20}$
3	1.342	$5.708 \cdot 10^{20}$	$5.715 \cdot 10^{20}$	$0.992 \cdot 10^{20}$
4	1.879	$7.328 \cdot 10^{20}$	$7.316 \cdot 10^{20}$	$1.395 \cdot 10^{20}$
5	2.416	$8.665 \cdot 10^{20}$	$8.688 \cdot 10^{20}$	$2.685 \cdot 10^{20}$
6	2.595	$9.768 \cdot 10^{20}$	$9.712 \cdot 10^{20}$	$4.986 \cdot 10^{20}$
7	3.490	$1.068 \cdot 10^{21}$	$1.075 \cdot 10^{21}$	$7.081 \cdot 10^{20}$
8	4.027	$1.143 \cdot 10^{21}$	$1.146 \cdot 10^{21}$	$6.536 \cdot 10^{20}$
9	4.564	$1.205 \cdot 10^{21}$	$1.193 \cdot 10^{21}$	$3.909 \cdot 10^{20}$
10	5.101	$1.256 \cdot 10^{21}$	$1.249 \cdot 10^{21}$	$1.833 \cdot 10^{20}$
11	5.638	$1.299 \cdot 10^{21}$	$1.332 \cdot 10^{21}$	$0.824 \cdot 10^{20}$
12	6.175	$1.334 \cdot 10^{21}$	$1.340 \cdot 10^{21}$	$0.296 \cdot 10^{10}$
13	6.712	$1.362 \cdot 10^{21}$	$1.317 \cdot 10^{21}$	$0.102 \cdot 10^{20}$
14	7.249	$1.386 \text{x} 10^{21}$	$1.392 \cdot 10^{21}$	$0.0538 \cdot 10^{20}$
15	7.786	$1.406 \cdot 10^{21}$	$1.187 \cdot 10^{21}$	$0.0302 \cdot 10^{20}$

For the case, which is given in the table 2, the initial data are precise enough. As it is clear from the table, monotone increasing profile is well reconstructed on depths up to ~ 6 mkm, and further, deviation increases. On the other hand, error estimation here is rather large, especially in the middle of the table, whereas at the end where deviation between computation and testing increase the error estimation is less than these deviations.

The carried out investigation of Fisher matrix and covariance matrix coming from probability function (13) – (15) shows that they are not always have performance of positive determination. With increase of number of items which are kept in formula (15) the number of negative diagonal elements of covariance matrix decreases. While keeping three last addendum in a asymptotic series (15) more variants at which Fisher matrix is positively determined are realized, and all diagonal elements of covariance matrix are positive. However analysis show, that not always it diagonal elements adequately reflect error of profile reconstruction. An example of this can be the table 2. With increase of number addendum which are kept in expression (15) the convergence of likelihood function has been taken place. Results which have been obtained for informational and covariance matrices contrast with this.

Presence of negative eigenvalue in Fisher matrix justifies that near the point of expected maximum of that approximation of likelihood function which we are investigating (the first derivatives are equal to zero) its profile in space of variables is not convex, and can have look saddles. To find it out, we have studied dependency of likelihood function from its variables near the expected maximum. In case of all studied profiles of impurity distribution density, the likelihood function had a convex parabolic character for some set of c_j, where $1 \le j \le j_{max} < n$, n is a task dimension. For $j > j_{max}$ likelihood function did not have such explicitly expressed convex look. These likelihood of j correspond to the most deep layers of the investigated sample, to which beam penetrates. Analysis of likelihood function and Fisher matrix shows that this region of the sample is objectively the less informative to obtain reliable results of reconstruction. Physically it means that contribution of X-Ray radiation from deep layers due to damping is considerably less then from surfaces, and it turns out to be insufficient for a rather precise determination of impurity in maximal depths on which beam can spread. For the correct solution of the appeared mathematical problems mentioned above, first of all, it is necessary to use the most suitable approximation for M_{ij} ! = $\Gamma(M_{ij} + 1)$ in $M_{ij} \le 1$.

4. CONCLUSIONS

1. The carried out investigations allow to explain "overshoot" of the reconstructed profile "pass" the testing one in that case when the yield of X-Ray radiation is calculated by formula (1) by means of thorough numerical integration. The reason is that maximum-likelihood algorithm has been developed for matrix equation (2) and not for the integral one (1).

2. The up-graded variants of likelihood function (13) -(15) have been offered and studied without a strict mathematical substantiation. Algorithm (9) which is offered in [1] and which do not comes from the investigated variants of probability function has been used for this. However, the increase of likelihood function for all its variants at all test profiles and different ways of calculation of yield of X-Ray radiation has been observed with its use. Convergence of series (15) which is used in likelihood function with increase of number of keeping addendum which contain B_i factors has been observed.

3. Informational and covariance matrices which correspond to different variants of probability function have been studied. Practical use of covariance matrix for error estimation of the profile restored with the stipulated variants of probability function turns out to impossible. The reason of this lies in the fact that in many of the investigated variants they did not have positive determination. And in those cases when this condition was fulfilling the obtained error estimations of profile reconstructed did not correspond to the really obtained. It points out on necessity of correct account of influence of deep layers of the investigated sample on forming of probability function and matrices which are following from it.

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ОЦЕНКА КАЧЕСТВА МЕТОДА МАКСИМАЛЬНОГО ПРАВДОПОДОБИЯ ПРИМЕНИТЕЛЬНО К ЗАДАЧЕ ОПРЕДЕЛЕНИЯ РАСПРЕДЕЛЕНИЯ ПРИМЕСИ ПО ХАРАКТЕРИСТИЧЕСКОМУ РЕНТГЕНОВСКОМУ ИЗЛУЧЕНИЮ, ВОЗБУЖДАЕМОМУ ПРОТОНАМИ

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Проведено численное исследование для разных приближений функции правдоподобия и матрицы Фишера применительно к алгоритму максимального правдоподобия для определения профиля примеси некоторого химического элемента в исследуемом образце методом PIXE. Показано, что проведенное ранее тестирование этого алгоритма указывает на принципиальную возможность его применения для восстановления профиля примеси методом PIXE, однако, его практическое применение вызывает трудности, а предложенное ранее выражение для функции правдоподобия не позволяет определить точность восстановления профиля примеси. Изучены проблемы, препятствующие возможности практического использования алгоритма.

ОЦІНКА ЯКОСТІ МЕТОДУ МАКСИМАЛЬНОЇ ПРАВДОПОДІБНОСТІ ПРИ ЗАСТОСУВАННІ ДО ЗАДАЧІ ВИЗНАЧЕННЯ РОЗПОДІЛУ ДОМІШКУ ПО ХАРАКТЕРИСТИЧНОМУ РЕНТГЕНІВСЬКОМУ ВИПРОМІНЮВАННЮ, ЩО ЗБУДЖУЄТЬСЯ ПРОТОНАМИ

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Проведено численне дослідження для різних наближень функції правдоподібності и матриці Фішера при застосуванні до алгоритму максимальної правдоподібності при визначенні профілю домішку якогось хімічного елемента в зразку, що досліджується методом PIXE. Показано, що проведене раніше тестування цього алгоритму вказує на принципову можливість його використання для встановлення профілю домішки методом PIXE, однак, його практичне використання визиває труднощі, а наведений раніше вираз для функції правдоподібності не дозволяє визначити точність встановлення профілю домішки. Досліджені проблеми, що перешкоджають можливому практичному використанню алгоритму.