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Information Characteristics of Analytical Signals at X-Ray Structure Analysis

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Abstract

Currently, in various industries, the improvement of technological processes becomes possible with the use of fast and accurate methods and means of continuous analysis of the composition and properties of gaseous, liquid and solid substances. The increasing requirements for the quality of raw materials and finished products, the improvement and development of new technological processes and the related tasks of managing these processes, the increasing requirements for environmental protection require further improvement of systems and devices for preliminary processing of information coming from the analyzing installation, designed to solve control problems composition and properties of substances. Such systems use a variety of analytical methods, the most common of which are spectrometry, adsorption, hydrochemical and thermal analysis methods. In particular, when conducting scientific research in the field of chemistry, biology, medicine, pharmacology, 40% of all methods of analysis of substances are spectrometric, 30% are adsorption, 10% are hydrochemical, 10% are thermal, and 10% is a group of 15 other analytical methods. The problem of operational control of environmental pollution has recently become especially relevant. In the air and water basins of a typical large city with petrochemical, metallurgical, electrical, oil refining industries, electrochemical production at many enterprises, there are more than 1900 organic compounds, about 30 inorganic compounds and heavy metals, toxic in their effect on the body. This article is devoted to the analysis of information characteristics of signals coming from spectrometric installations.

KEY WORDS: *spectrometry, devices for preliminary processing of information, X-ray methods of analysis.*

I. INTRODUCTION

As you know, the X-ray detector accepts those of them, phases

which coincide, which is described by the Bragg - Wolfe law (Fig. 1):

$$2d \sin \Theta = n\lambda; \quad (1)$$

where n - is an integer;

d - is the distance between the reflection planes;

Θ - is the angle between the incident ray and the direction of the plane.

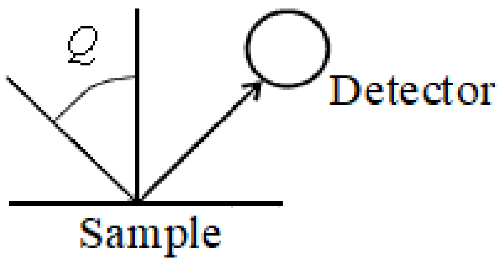

Fig. 1. X-ray structural analysis scheme

For a spectrum of the 1-st order (*n = 1*) and at constant Θ, the number of reflectedwaves with a length λ is proportional to the number of planes satisfying (1).

Thus, the intensity of the reflected radiation at the wavelengthλ_1 will be determined by the intensity of the distribution density function*f(d)* on the argument *d1* (λ_1, d_1 satisfy (1)). Thus, to determine the distribution density of the signal *f (λ)*, it is sufficient to determine *f(d)*.

In fact, the function *f(λ)*, as well as the function *f(d)*, is a function of a discrete argument (the set of values *λ, d* is determined based on (1)).

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However, in order to use the apparatus of the theory of probability, at certain stages, we will consider it a function of a continuous argument (extrapolating it to the region of forbidden values λ or d).

RESULT AND DISCUSSION

Let us consider this problem in relation to different types of crystal lattice.As you know, there are seven such types in total, the simplest of which isis the cubic system. It is also known that for it the interplanardistances are determined by the formula [1]:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}};$$

where$a$ - is the interatomic distance,

h, k, l - small integers (plane indices).

The ratio of d values for planes with different indices should be determined by the series 1: $\frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} : \frac{1}{\sqrt{4}} : \frac{1}{\sqrt{5}}$.....

In this case, we can assume that the quasi-continuous distribution d - is determined by the distribution of the function

$$d = \frac{1}{\sqrt{x}},$$

where$x$ - is a continuous random variable with a uniform distribution law

x=Aat $x \in (x_{\min},\ x_{\max})$.

Then the distribution density d is described by the function

$$f(d)\frac{A}{d^2}\ \ when\ d \in \left(\frac{1}{\sqrt{x_{\max}}}, \frac{1}{\sqrt{x_{\min}}} \right).$$

Thus, the signal distribution density in this case is described by a monotonically decreasing function.

The most difficult task seems to be for the three-wedge system.

In this case, the expression for $\sin^2 \Theta$ has the following form [1]:

$$\sin^2 \Theta = \frac{\lambda^2}{4}\left[h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2klb^* c^* \cos\alpha^* + 2lhc^* a^* \cos\beta^* + 2hka^* b^* \cos\gamma^*\right], \quad (2)$$

wherea^*, b^*, c^* - lengths of edges of a unit cell in reciprocal space; $\alpha^*, \beta^*, \gamma^*$ - angles between the edges of a unit cell in reciprocal space.

Having determined the distribution law $sin^2\Theta$, it is easy to determine the distribution law d based on (1):

$$d = \sqrt{\frac{\gamma^2}{4\sin^2\Theta}} = \frac{1}{\sqrt{\left[h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2klb^* c^* \cos\alpha^* + 2lhc^* a^* \cos\beta^* + 2hka^* b^* \cos\gamma^*\right]}}. \quad (3)$$

In function (3), the arguments are $h, k, l,$ which, as in the previous case, will be considered continuous quantities with a uniform distribution law, as well as the quantities a^*, b^*, c^* and $\alpha^*, \beta^*, \gamma^*$.

Usually the values $\alpha^*, \beta^*, \gamma^*$ vary within small limits, and can be considered [2] $\cos\alpha^* \approx 1,\ \cos\beta^* \approx 1,\ \cos\gamma^* \approx 1$.

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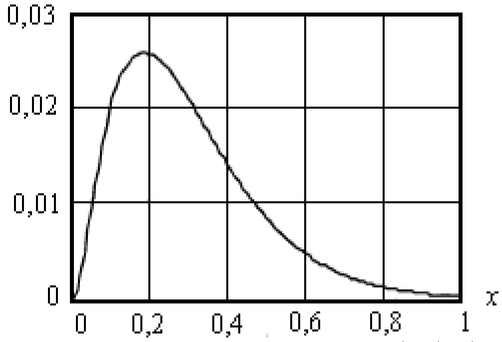
The quantities a^*, b^*, c^* can be considered as having an asymmetric distribution close to the Poisson distribution [2] shown in Fig. 2.

Let us now consider the problem of analyzing the distribution density of the function (3).



Rice.2. Distribution of parameters a^*, b^*, c^*.

The function shown in Fig. 2 for further use it is convenient to approximate near

$$f_1(x) = a_1 x + a_2 x^2 + a_3 x^3; \qquad (4)$$

In this case, the domain of definition $x \in (0,1)$.

Obviously, the normalization condition for the distribution must be satisfied

$$\int_0^1 f_1(x)dx = 1.$$

Consider the distribution of the product of two quantities, one of which has Poisson (4), and the other has a uniform distribution of the form

$$f_2(x) = 1.$$

Applying the formula for the product of random variables

$$g(z) = \int_{1/z}^{1} \frac{1}{x} f_1(x) f_2\left(\frac{z}{x}\right) dx,$$

we get

$$g_1(x) = a_1 + \frac{a_2}{2} + \frac{a_3}{3} - a_1 x - a_2 \frac{x^2}{2} - a_3 \frac{x^3}{3} = b_0 + b_1 x + b_2 x^2 + b_3 x^3; \quad (5)$$

For example, let's take numerical values

a_1=11,94, a_2=20,5, a_3=9,48.

For the chosen values of a_1, a_2, $a_3$we obtain

b_0=3,21, b_1=-7,9, b_2=6,785, b_3=-2,l.

Function (5) with such values of the coefficients has the form of a decaying exponent (Fig. 3)

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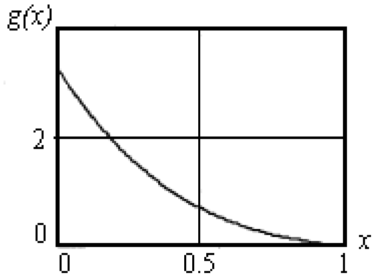

Fig. 3 The form of the exponential function *g(x)*

The distribution of the function

$y=x^2$.

Applying the notation and indexing similar to the notation used in [1], we obtain:

$$y=\varphi(x)=x^2;\ \ x=\psi(y)=\sqrt{y};\ \ \psi'(y)=\frac{1}{2\sqrt{y}};$$

$$g_2(y)=f[\psi(y)]|\psi'(y)|=\frac{1}{2}\left[\frac{b_0}{\sqrt{y}}+b_1+b_2\sqrt{y}+b_3y\right]. \quad (6)$$

Distribution (6) has the form shown in Fig. 4.

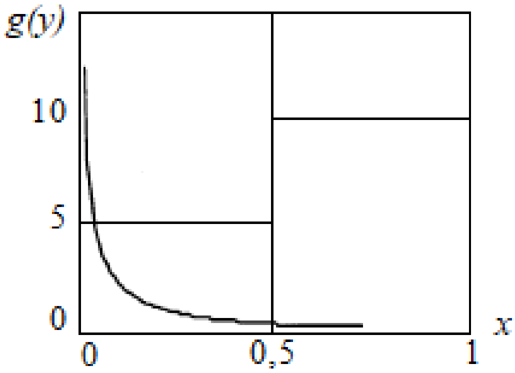

Fig. 4. View of the distribution function (6)

Obviously, the distributions of quadratic terms h^2a^{*2}, k^2b^{*2}, l^2c^{*2} in expression (2), as well as other termsthis expression, since they are also works,which, as shown above, are characterized by hyperbolic distributions.

Let us now consider the distribution of the sum of functions

$y_1, y_2, \ldots,$

each of which has a distribution of the form (6).

For the analytical solution of this problem, we use the approximation function (6) function

$$g_2(y)=ae^{-\alpha_y}.(7)$$

functions (6) and (7) somewhat differ from each other at the boundaries of the definition interval, but inside it they are close.

Consider the problem of determining the distribution of the sum of quantities

$$z=y_1+y_2,$$

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havingdistributions

$$f_1(y_1) = ae^{-\alpha y_1}; \;\; f_2(y_2) = ae^{-\alpha y_2};$$

coefficient$a$ is determined from the condition for normalizing the distribution

$$a\int_0^1 e^{-\alpha y}dy = 1;$$

fromhere

$$a = \frac{\alpha}{1-e^{-\alpha}} \approx \alpha;$$

Fromthisweget

$$f(z) = \int_{-\infty}^{\infty} f_1(y_1) f_2(z-y_1)dy_1;$$

due to the fact that outside the domain of definition, the distribution functions are equal to zero

$$f_1(y_1) = 0 \;\; at \;\; y_1 < 0,$$
$$f_2(z-y_1) = 0 \;\; at \;\; z < y_1,$$

then for the domain of definition $z \in (0,1)$ we obtain:

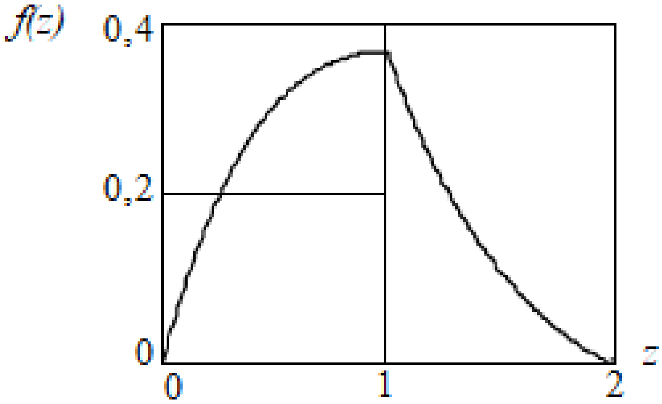
$$f(z) = \int_0^z f_1(y_1) f_2(z-y_1)dy_1 = a^2\int_0^z e^{-\alpha y_1}e^{-\alpha(z-y_1)}dy_1 = a^2 ze^{-\alpha z}.$$

For the domain of definition $z \in (1,2)$, we obtain

$$f(z) = \int_{z-1}^{1} f_1(y_1) f_2(z-y_1)dy_1 = a^2(2-z)e^{-az}.$$

A typical form of the distribution law of this function is presented in fig. 5.

Obviously, the composition of four more random variables has a distribution law close to normal, which also follows from the limit theorem of probability theory [3,4].



Rice. 5. Form of the distribution function $f(z)$

It is now easy to show that the distribution law of the function where z - is a random variable having a distribution law close to normal, with a mathematical expectation $m_z=0,5$, and a mean squaredeviation σ=1/3, on the interval $z \in (0,1)$ (which determines the interval $z_1 \in (\infty,1)$) close to hyperbolic.

Thus, the distribution law (3) of the parameter d is also close tohyperbolic.

CONCLUSION

Hence it follows that the distribution of the X-ray radiation intensity is close to the same law.

Thus, regardless of the analytical method used in analytical measurements, the a priori level distribution law signals is close to logarithmically - uniform, which allows you to build unified means of transformation of analytical signals with an optimal scale of their quantization [5].

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