Application of the Compton Effect to Solve Problems of Condensed Matter Physics

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The prospects for the application of X-ray spectral methods and scattering phenomena as a basis for chemical and phase analysis in new areas are considered. It is theoretically shown that the sensitivity of the scattering method does not depend on the structure and quality of the sample surface and increases sharply with a decrease in the atomic number of the analyzed impurity. The sensitivity of the method is analyzed in the study of multicomponent standards of stoichiometric composition based on H, Li, B, C, O and F, and compared with the sensitivity of traditional analytical methods. The concentration sensitivity of detecting the content of light impurities in metals is calculated and experimental confirmation is given for titanium-hydrogen and iron-carbon systems. For the first time, the Compton method is generalized for the analysis of multicomponent systems of unknown composition. To do this, using the Duvauchelle approach, the concept of the effective atomic number by the scattering property is introduced. It is shown that the dependence of the effective atomic number on the parameter x, which reflects the measurement conditions (scattering angle and primary radiation wavelength), uniquely determines a multicomponent compound. Based on the sensitivity analysis, the range of application of the scattering method is substantiated. From the side of small values of the parameter x, the method is limited due to Bragg reflections superimposed on the Rayleigh peak. For large values of the parameter x, the sensitivity of the method decreases due to the large discrepancy between the intensities of coherent and incoherent scattering. The examples of solving analytical problems are given, in which the use of X-ray fluorescence and diffraction analysis is either very difficult or impossible at all.

Keywords: Rayleigh-to-Compton scattering intensity ratio, Effective atomic number, Light elements, Stoichiometric compounds.

1. INTRODUCTION

Traditional X-ray methods of material analysis are based on the phenomena of diffraction and fluorescence. Scattering is usually considered a background signal, so is not used for analytical purposes. At the same time, much attention has recently been paid in the literature to the application of the scattering phenomenon to the study of chemical elements with a small atomic number. Such a study is possible due to the Compton effect on bound electrons of an atom [1]. In this work, the Compton scattering method (its sensitivity and range) is theoretically investigated, and examples of its modern applications are given.

2. ESSENCE OF THE METHOD

Compton scattering is a phenomenon of inelastic scattering of photons by free charged particles. The Compton effect is similar in nature to the photoelectric effect; the difference is that with the photoelectric effect, the photon is completely absorbed by the electron, while with Compton scattering it only changes the direction of motion and energy (wavelength). The change in the wavelength of a photon after interaction with a free electron is described by the Compton formula:

$$\Delta\lambda = \frac{h(1-\cos 2\theta)}{m_e c}, \qquad (1)$$

where m_e is the electron mass, h is Planck's constant, c is the speed of light, 2θ is the scattering angle.

If an electron by which a photon is scattered is in the atom, then the scattering pattern becomes more compli-

cated. Let us consider monochromatic X-rays with photon energies from 9 to 22 keV. This range falls within the characteristic region of the binding energies of electrons in the atom. If the energy of the incident photon is less than the binding energy of the electron with the nucleus, then the electron is not knocked out of the shell and the atom as a whole scatters the photon. In this case, instead of the mass of the electron in the denominator of formula (1), there will be the mass of the atom, which is tens of thousands of times larger, which means that the change in the wavelength will be tens of thousands of times smaller. The amplitude of coherent scattering is described by the atomic scattering function or atomic form factor f, which is the ratio of the amplitude of radiation scattered by an atom to the amplitude of radiation scattered by one free electron [2].

At small scattering angles, the value of the atomic form factor approaches the number of electrons in the atom, but as the scattering angle increases, it rapidly decreases due to the interference of contributions from different parts of the atom [3]. When the energy of the incident photon is much greater than the binding energy, we can assume that the electron is free, and the scattering is described by the scattering formulas for a free electron. The probability of excitation of an atom, when part of the photon energy is transferred to an electron, is described by the incoherent scattering function S [2]. In the literature, the incoherent scattering function of a multi-electron atom is usually assumed to be the product $Z \cdot S$, where Z is the atomic number of the chemical element. Consequently, the Compton photon has a larger wavelength, since part of the energy of the incident photon is spent on knocking the electron out of

the shell and giving it kinetic energy.

Different electron shells of an atom scatter independently of each other, i.e., the scattering intensity is a simple sum of scattering by different electron shells. The lower the binding energy of an electron in an atom, the greater its contribution to Compton scattering. For a multi-electron atom with different electron binding energies, some electrons will scatter in the Compton type, while others will scatter in the Rayleigh type. Each electron interacts with only one photon, so, according to [3], the following approximation is valid for atoms with $Z < 20$:

$$S(x, Z) = Z - \left[f(x, Z) \right]^2. \tag{2}$$

The incoherent scattering function S and the atomic form factor f are complex functions of the element's atomic number, the scattering angle, and the wavelength of the scattered radiation. In the literature, the parameter $x = \dfrac{\sin \theta}{\lambda}$ (the momentum transfer variable) is used as an argument. The numerical values of these functions for all chemical parts are given in [4].
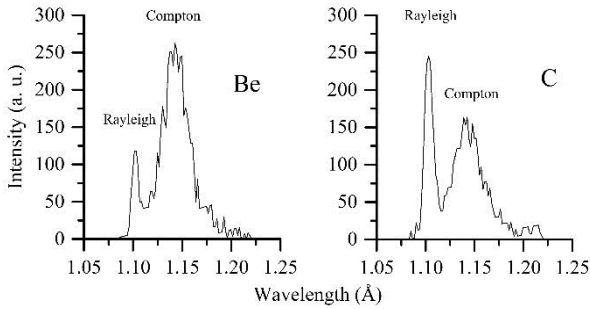
Fig. 1 – Fragments of experimental scattering spectra. Materials of scatterers are beryllium and carbon

The fact that the scattering spectrum (Fig. 1) consists of only two peaks is the fundamental difference from the diffraction and fluorescence spectra. The position of these peaks is determined by the wavelength of photons of coherent (Rayleigh) and incoherent (Compton) scattering, that is, it does not depend on the type of atoms that make up the substance (Moseley's law) or on their relative position (Bragg's law). The intensity of these peaks is determined solely by the number of Rayleigh and Compton photons, so it indicates how many electrons have a binding energy greater than that of the primary X-rays. The ratio of Compton and Rayleigh scattering intensities has a unique property: it sharply increases with decreasing atomic number of the scatterer.

Fig. 1 shows two fragments of the experimental spectra. Even for chemical elements close in atomic number, an increase in the intensity of the Compton component and a decrease in the Rayleigh component are obvious. This difference is due to the fact that carbon has 20 % more electrons than beryllium. Thus, the method is very promising for the study of light chemical elements that do not have many electrons and the contribution of each of them is significant. In general, the use of scattering makes sense for the identification

of chemical elements with atomic number from $Z = 12$ (magnesium) to $Z = 1$ (hydrogen), where it is difficult to apply X-ray fluorescence analysis due to the absorption of long-wavelength radiation and low fluorescence yield [5].

3. SENSITIVITY OF THE METHOD

Since Rayleigh and Compton scattering are independent of each other, according to Sommerfeld [6], the one-electron problem for the hydrogen atom is generalized to the case of a set of different atoms by summing the intensities:

$$R(C, Z, x) = \frac{I_C}{I_R} = \frac{\sum_i C_i S_i (Z_i x)}{\sum_i C_i f_i^2 (Z_i x)}. \tag{3}$$

The numerator and denominator of formula (3) are represented by additive functions $S_i(Z_i x)$ and $f_i^2(Z_i x)$ respectively. Let us analyze this dependence in a general form using the representation for the incoherent scattering function $S_i(Z_i x)$ and coherent scattering $f_i^2(Z_i x)$ for an element with atomic number Z_i. The measurement sensitivity of any chemical element in a material is determined by the partial derivative of function (3) with respect to the concentration C_i

$$\frac{\partial R}{\partial C_i} = \frac{1}{\left(\sum_i C_i f_i^2 (Z_i, x) \right)^2} \times \tag{4}$$
$$\times \left(S(Z_i, x) \sum_i C_i f_i^2 (Z_i, x) - f_i^2 (Z_i, x) \sum_i C_i S_i (Z_i, x) \right)$$

$$\frac{\partial R}{\partial C_i} = \frac{1}{\left(\sum_i C_i f_i^2 (Z_i, x) \right)^2} \times \left(S(Z_i, x) - f_i^2 (Z_i, x) R(C_i Z_i x) \right). \tag{5}$$

Equation (5) makes it possible to calculate the change in the signal (the ratio of the peaks of incoherent and coherent scattering $R_i(C_i Z_i x)$ with a change in the atomic fraction C_i of an impurity with atomic number Z_i in a cluster of atoms. Graphically, this dependence is shown in Fig. 2.
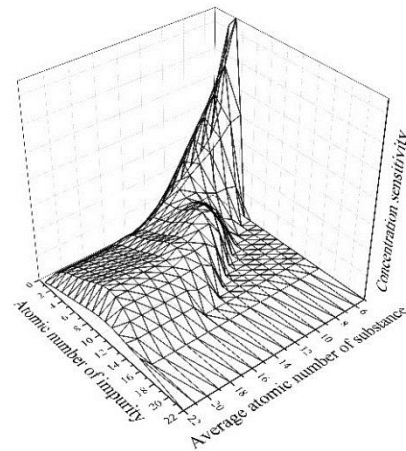
Fig. 2 – Concentration sensitivity in the determination of an impurity with atomic number Z_i in a multicomponent material with average atomic number Z

From relation (5) and Fig. 2, the following conclusions can be drawn.

- The lower $\sum_i C_i f_i^2(Z_i, x)$, the higher the sensitivity of the determination of any chemical element, i.e., the lower the average atomic number of chemical elements in the cluster.

- The sensitivity of determining a chemical element with atomic number Z_i is the higher, the greater the difference between the ratio $\dfrac{S_i(Z_i, x)}{f_i^2(Z_i, x)}$ for this element and the analytical signal $R(C, Z, x) = I_C/I_R$ the entire cluster.

- It is possible to calculate Z and x for which $\dfrac{\partial R}{\partial C_i} = 0$ $\frac{\partial R}{\partial C_i} = 0$, i.e., this method for determining chemical elements degenerates.

The conclusions drawn indicate that, first, the method is promising for compounds of light chemical elements; this will be discussed in detail later. Second, the lighter the impurity and the heavier the matrix, the higher the sensitivity. Therefore, the method is very promising for detecting light impurities in metals. This is especially pronounced in metal-hydrogen systems, in which it is possible to reach the limit of detection at the level of $10^{-4} \div 10^{-3}$ mas %. The theoretical calculation of the increase in the signal value $\Delta R(C, Z, x)$ as a percentage per one percent increase in the impurity concentration (concentration sensitivity) is given in Table 1.

Table 1 – Calculated value of the concentration sensitivity (%) when measuring light impurities in metals by the ratio of the integral intensities of the Compton and Rayleigh peaks

Impurity	Metal						
	Ti	Fe	Ni	Zr	Nb	Ag	W
H	16.52	20.70	22.30	125.25	153.88	–	–
He	3.63	3.95	4.02	5.68	5.74	6.50	11.66
Li	2.47	2.66	2.70	3.64	3.67	4.05	6.18
Be	2.16	2.32	2.36	3.15	3.18	3.49	5.14
B	1.96	2.12	2.16	2.89	2.92	3.20	4.64
C	1.89	2.05	2.09	2.83	2.85	3.13	4.51
N	1.70	1.85	1.90	2.58	2.60	2.86	4.09
O	1.55	1.70	1.75	2.40	2.42	2.65	3.78

An experimental verification of this statement was carried out on standard samples of the titanium-hydrogen binary system. The obtained concentration sensitivity value of 170 mass % turned out to be even higher than the calculated ones, although the reason for this has not yet been clarified. For the Fe-C system, the value of the concentration sensitivity corresponds to the calculated value and is 2.1 % per 1 mass % of carbon, which is quite sufficient to measure this impurity with an accuracy of 0.05 mass %.

4. COMPARISON WITH OTHER ANALYTICAL METHODS

For a numerical evaluation, we compare the sensitivity of the Compton scattering method with gravimetric analysis based on determining the mass of a substance. Gravimetric analysis is one of the most versatile methods. A significant advantage of this method is the high accuracy of the analysis. The usual error of gravimetric determination is 0.1-0.2 %. Its sensitivity is constant and depends only on the atomic weight:

$$\frac{\Delta M}{M} = \frac{\Delta n_j A_j}{\sum_j^m n_j A_j}.$$

To compare the methods, we will take chemical compounds of light chemical elements with a known composition as a model of a material with an impurity. The atomic form factor and the incoherent scattering function are almost identical to the atomic (molecular) weight. These are also additive functions for the accumulation of atoms of different chemical elements or molecules. This significantly simplifies data processing, since there is no mutual influence of impurities, as in X-ray fluorescence analysis. So, let us rewrite formula (3) taking into account (2) for a cluster of n atoms, according to [6]:

$$R = I_C / I_R = \frac{\sum_i n_i \left(Z_i - \sum_k f_{ik}^2\right)}{\sum_i n_i \left(\sum_k f_{ik}\right)^2}. \tag{6}$$

Considering that

$$\left(\sum_k f_{ik}\right)^2 = \sum_k f_{ik}^2 + 2\sum_{k \neq k'} f_{ik} f_{ik'},$$

$$\sum_k f_{ik}^2 = \left(\sum_k f_{ik}\right)^2 - 2\sum_{k \neq k'} f_{ik} f_{ik'},$$

one can write:

$$R = \frac{\sum_i n_i Z_i}{\sum_i n_i \left(\sum_k f_{ik}\right)^2} - \frac{\sum_i n_i \left(\sum_k f_{ik}\right)^2}{\sum_i n_i \left(\sum_k f_{ik}\right)^2} + 2\frac{\sum_i n_i \sum_{k \neq k'} f_{ik} f_{ik'}}{\sum_i n_i \left(\sum_k f_{ik}\right)}.$$

For the chosen Z range, we have: $f_{ik} = f_{ik'} = f_i$ and $k = 2$ (2 electrons per level), then [3]:

$$R = \frac{\sum_i n_i Z_i}{4\sum_i n_i f_i} - 1 + 2\frac{2\sum_i n_i f_i^2}{4\sum_i n_i f_i^2} = \frac{1}{4}\frac{\sum_i n_i Z_i}{\sum_i n_i f_i^2}. \tag{7}$$

According to equation (7), the sensitivity of the Compton scattering method depends on the ratio of the sums of atomic weights and atomic form factors of all atoms of the compound:

$$\frac{\partial R(x)}{\partial n_i} = \frac{1}{4}\frac{Z_i \sum_{i=1}^m n_i f_i^2 - f_i^2 \sum_{i=1}^m n_i Z_i}{\left(\sum_{i=1}^m n_i f_i^2\right)^2}, \tag{8}$$

where m is the number of types of atoms in the compound. The results of calculations obtained using numerical data [4] are shown in Table 2.

Thus, the theoretical calculation proves that the scattering method is more sensitive than gravimetric analysis. Its sensitivity depends on the measuring conditions and increases with decreasing $\sin\theta/\lambda$. Now consider the range of application of the scattering method.

5. RANGE OF APPLICATION

The analytical signal $R(Z,x) = I_C/I_R$ is a function of two arguments. Let us first define the parameter $x = \sin\theta/\lambda$. Therefore, to measure the intensity of Rayleigh scattering, it is important that there are no Bragg reflections in the spectrum, since they have the same wavelength as the coherent scattering component. The intensity of the diffraction peaks sharply decreases with increasing x according to the law $\exp\left(-const\left(\dfrac{\sin\theta}{\lambda}\right)^2\right)$ due to the violation of the order of the positions of atoms in the lattice nodes (thermal vibrations, statistical curvature). For most substances, with the exception of single crystals, there are no Bragg reflections already at $x > 0.6\,\text{Å}^{-1}$ [2]. In addition, at $x > 2\,\text{Å}^{-1}$, the intensity of incoherent scattering is many times greater than the intensity of coherent one, which leads to an increase in the measurement error of the intensity of the Rayleigh peak.

To determine the range of chemical elements (atomic numbers Z), we consider a graphical representation of the data [4] at a fixed value of the parameter $x = 1.15\,\text{Å}^{-1}$ (Fig. 3). For chemical elements with $Z < 7$ (N), the ratio $\dfrac{S(Z)}{f(Z)^2}$ decreases sharply, because as Z increases, the electrons become more bound, and the charge density increases at smaller values of r (orbital radius), which contributes to an increase in the fraction of the coherent component of the scattered radiation [3]. Starting from oxygen ($Z = 8$) (at $x < 0.8\,\text{Å}^{-1}$), the influence of L-electrons sharply slows down the decay of the dependence and we observe a plateau, which was experimentally found by Wollan [7]. In this section, the derivative of the function $\dfrac{S(Z)}{f(Z)^2}$ is close to zero, which negatively affects the sensitivity of the method in this range. In the section from Na ($Z = 11$) to S ($Z = 16$), when the levels (1, 0), (2, 0) and (2, 1) are already filled with K- and L-electrons, orbitals with M-electrons begin to form. An increase in the distance from the electrons to the center of the atom contributes to a decrease in the charge density and, accordingly, to an increase in the fraction of the incoherent component of the scattered radiation; as a result, a second sloping part of the curve is observed.
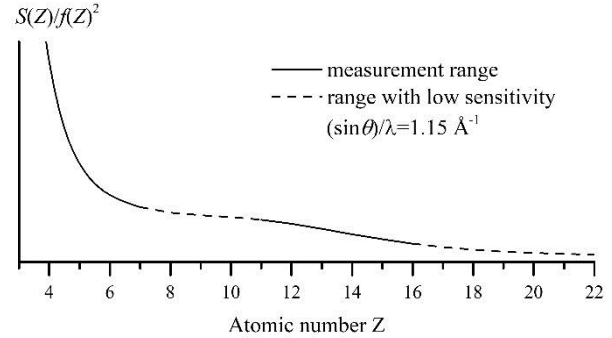
Fig. 3 – Function $\dfrac{S(Z)}{f(Z)^2}$ at a fixed value $\dfrac{\sin\theta}{\lambda} = 1.15\,\text{Å}^{-1}$ according to [4]

According to Fig. 3, for atoms with $Z > 16$, the fraction of incoherent scattering is so small that the application of the Compton scattering method becomes inexpedient.

Thus, for $x = 1.15\,\text{Å}^{-1}$, two ranges of atomic number values can be determined, in which the dependence $\dfrac{S(Z)}{f(Z)^2}$ meets the requirements for the calibration function: from $Z = 1$ (H) to $Z = 7$ (N) and from $Z = 11$ (Na) to $Z = 16$ (S). And if the second range is successfully covered by X-ray fluorescence spectral analysis, then the first one is of considerable interest.

Table 2 – Numerical evaluation of the sensitivity of the Compton scattering method and gravimetric analysis; change in the amount of impurity in one atom

Compound	Element	$\partial R(x)/\partial n_i$					$\Delta M/M$
		$x = 0.7\,\text{Å}^{-1}$	$x = 0.8\,\text{Å}^{-1}$	$x = 0.9\,\text{Å}^{-1}$	$x = 1.2\,\text{Å}^{-1}$	$x == 1.5\,\text{Å}^{-1}$	
Li_2CO_3	Li	0.054	0.067	0.080	0.133	0.222	0.094
	C	0.090	0.107	0.126	0.211	0.364	0.163
	O	0.121	0.140	0.162	0.251	0.404	0.217
LiF	Li	0.125	0.154	0.188	0.311	0.492	0.268
	F	0.402	0.453	0.498	0.622	0.729	0.732
B_4C	B	0.087	0.101	0.116	0.157	0.053	0.196
	C	0.108	0.123	0.139	0.153	–	0.217
C_2H_6O	C	0.115	0.127	0.140	0.179	0.184	0.261
	H	0.031	0.037	0.044	0.076	0.135	0.022
	O	0.171	0.187	0.203	0.232	0.130	0.347
H_2O	H	0.075	0.089	0.104	0.160	0.255	0.056
	O	0.431	0.473	0.514	0.648	0.754	0.888
$Li_2B_4O_7$	Li	0.018	0.022	0.026	0.046	0.080	0.041
	B	0.027	0.031	0.036	0.055	0.084	0.064
	O	0.049	0.055	0.061	0.079	0.089	0.095
B_2O_3	B	0.064	0.074	0.085	0.130	0.201	0.155
	O	0.114	0.128	0.143	0.190	0.223	0.230

The study of this range is an urgent task for many areas of science and technology, namely, the compounds of elements H, C, O, N are the basis of living nature; elements H, C and O form the base of the fuel, and Be and B are part of the promising structural materials.

6. APPLICATION OF THE COMPTON SCATTERING METHOD

Let us consider works, where the scattered radiation is used as the main parameter for solving analytical problems. In the previous section, it was shown that these are works devoted to the determination of elements with low atomic numbers. The use of fluorescent radiation in these cases is either very complicated or even impossible. As has already been established, this is primarily due to the low fluorescence yield, and in some cases, the impossibility of measuring the X-ray spectrum, for example, when determining the hydrogen content.

6.1 Study of One-Component Materials

One of the first is the work [8], which shows the possibility of determining the ratio of carbon and hydrogen in oil products. To do this, the authors used the ratio of the intensities of the coherently and incoherently scattered characteristic radiation of the tungsten anode of the X-ray tube (WL_a). The method has found wide application in the field of ecology. Known works are devoted to the use of the intensity of scattered radiation in the determination of various elements in water and other organic compounds, as well as water in soils for agricultural purposes. In [9, 10], various practically important cases were considered in detail, in which the incoherent component of the scattered primary radiation was mainly used and turned out to be a very sensitive parameter for this type of problems. We also note works, where the intensities of coherently and incoherently scattered radiation or the ratios of these intensities were used to determine the coating thickness [11, 12].

6.2 Study of Multicomponent Materials

We reviewed the study of the content of known impurities in a known matrix. When the prototype is an unknown multicomponent compound, the task becomes more difficult, because the same value of the analytical signal can correspond to several different compounds at once. The solution to this problem is described in the work of Duvauchelle [13], in which the concept of effective atomic number is introduced for multicomponent compounds. The author proves that the most correct among the existing definitions of this parameter is the consideration of a cluster of different atoms (compounds) as a chemical element in which the number of electrons per atom is equal to the number defined as the effective atomic number Z_{eff}.

In [14, 15], results were obtained that indicate the possibility of using the method to characterize human tissues. This makes it possible to study the histological features associated with the elemental composition. In [14], it was suggested that a change in the absorption of glucose by malignant cells can lead to the fact that these tissues will have an increased electron density.

The electron density was measured by the ratio I_C/I_R. The system was calibrated using solutions with known electron density. The results of a study of 22 tissue samples are presented, including four different classifications: adipose, malignant, fibroadenoma, and fibrocystic changes. In [15], Compton and Rayleigh scattering radiation from normal (adipose and fibroglandular), benign (fibroadenoma) and malignant (ductal carcinoma) breast tissues was measured at one value of the parameter $x = 0.99$ Å^{-1}. The results show that there are differences in the distribution of tissue effective atomic numbers, which are related to carbon ($Z = 6$) and oxygen ($Z = 8$) content in each type of the tissue.

In [16], Z_{eff} values for alloys were determined by interpolating the Z_{eff} dependence using data for neighboring elements. In [17], a practical method for identifying binary oxides by the dependence on Z_{eff} was proposed using a priori information about one of the elements, oxygen. The authors claim that this method can be applied to any material with a known content of various elements in the compound.

The ratio of coherent to Compton scattering intensities depends only on the composition of the mixture and provides the measurement of some complex functions of the atomic number Z and Z_{eff}. In order to measure the effective atomic number for Sb_2O_3, BaO, La_2O_3, CeO_2 and Nd_2O_3, the linear differential scattering coefficients of 59.5 keV γ-rays were studied using a high-resolution Si (Li) semiconductor detector. In [18], a similar approach was used to determine the effective atomic number of three-component standard mixtures $Al + Al(OH)_3$; the passport data of a standard sample on the aluminum content in the mixture were used. The requirement to have a priori information about the impurity content greatly narrows the limits of application of the method.

Using the Duvauchelle approach, in [18], the effective atomic number was determined from the condition that a single-component material has an interpolated atomic number Z_{eff}, for which equation (3) gives the same ratio $R(Z,x) = I_C/I_R$ as for a multicomponent compound. Since the incoherent scattering function and the atomic scattering factor depend on $x = \sin\theta/\lambda$, for a cluster of atoms, a certain value of $\sin\theta/\lambda$ corresponds to a certain value of the effective atomic number. It was experimentally proved [18] that when the measurement conditions, namely the wavelength or the scattering angle, change, the value of the effective atomic number determined in this way will also change. The dependence of the effective atomic number on $\sin\theta/\lambda$ is an important characteristic of a set of atoms of different types, which uniquely determines a multicomponent system and can be used as a calibration function.

In [19], the possibility of direct quantitative X-ray spectral determination of carbon, hydrogen, and oxygen in organic compounds consisting of these parts was shown. Due to the complexity of the task, the measurement had to be limited to only two values of the parameter $x = \sin\theta/\lambda$. As analytical parameters in the regression equations, the authors of [19] used the ratio

of the intensities of coherently and incoherently scattered lines of copper and palladium. The resulting calculated calibration dependences were used to assess the correctness of the analysis using models of various organic compounds: starch, glucose, butyl alcohol, citric and oxalic acids, etc. Experimental verification was carried out on a Spectroscan MAKS-GV X-ray scanning spectrometer with a BKhV-17 X-ray tube (Pd anode), in the spectrum of which the copper line is strongly pronounced. The test showed satisfactory results of the determination of H, O and C by the proposed method.

A wide range of samples was studied in [20]. The measurement was performed using the scattering spectra of standard one-component samples of beryllium, boron, and carbon, as well as multicomponent standards of stoichiometric compositions based on H, Li, B, C, O, and F. Materials in different structural states were used for the experiment: from liquid (H_2O and C_2H_6O) to coarse-grained polycrystals (LiF). Thus, it was experimentally shown that the scattering method is effective for studying substances in any structural state, since scattering occurs precisely on atoms.

Multicomponent compounds were identified by the calibration function $Z_{eff}(x)$, which was experimentally studied in the range $0.755 \text{ Å}^{-1} \leq x \leq 1.671 \text{ Å}^{-1}$. To ensure this range of x, the samples were irradiated with photons with energies of 9.88, 10.98, 11.22, 12.49, 14.95, 16.73, 17.47, 19.60, 22.16 keV. The calibration functions were smooth lines without peaks, which differed noticeably in shape and slope even for compounds with similar compositions. Their slope depended on the difference in the atomic numbers of the constituents of the compound: the greater the difference, the steeper the dependence. For example, for B_4C, the calibration function was almost the same as for a single-component material – parallel to the abscissa axis.

Therefore, the possibility of revealing a given phase in a mixture using the base of calibration functions, i.e., carrying out phase analysis due to the expansion in terms of the basis of smooth functions, has been experimentally shown. This opens up prospects for the use of X-ray analysis in biology and medicine – the identification of organic compounds in biological tissues: for example, the diagnosis of tumors before their actual manifestation by changing the phase composition of the tissue.

Control of the distribution of light parts over the depth of the standard is considered in [21]. The idea of improving the research method described in [20] is to change the thickness of the information layer and experimentally obtain the dependence of the impurity concentration on this thickness.

In the experiment, the depth of penetration of radiation into the material changes when the standard is rotated through an angle α (Fig. 4). An X-ray tube with a molybdenum anode illuminates the sample surface through a collimator. The sample is mounted on a goniometer and can be rotated using a lever with microscrews in the range of angles α from $-26°$ to $-5°$. The scattered radiation passes through the Soller collimator with an angular divergence of $0.2°$ and is reflected from the monochromator (HOPG), and then enters the scintillation detector through the second Soller collimator.
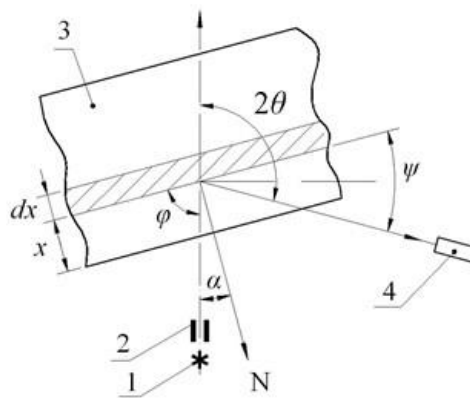
Fig. 4 – X-ray optical scheme. N is the normal to the sample surface, 2θ is the scattering angle, φ and ψ are the angles of incidence and exit of radiation; 1 – radiation source, 2 – collimator, 3 – sample on a goniometer, 4 – block of a crystal-diffraction spectrometer

The positions of the radiation source (pos. 1 and 2) and the positions of the system that registers the signal (pos. 4) remain fixed, and only the sample rotates (pos. 3). Thus, the angles of incidence φ and exit ψ of the radiation change, which ensures a change in the thickness of the information layer, and the scattering angle remains unchanged and amounts to $2\theta = 116°$. The results of the study are in good agreement with the results of cross-sectional metallography.

7. CONCLUSIONS

The ratio of intensities of Compton and Rayleigh scattering has a unique property – it sharply increases with decreasing atomic number of the scatterer. In the study of multicomponent materials, the sensitivity of the method is higher when determining the content of a light impurity in a heavy matrix. Within these limits, the sensitivity of the scattering method is not inferior to gravimetric analysis.

The use of the scattering phenomenon as a basis for the study of multicomponent systems opens up new areas of application of X-ray methods; the range of their use expands not only towards a decrease in the atomic number of a chemical element down to hydrogen, but also makes it possible to study multicomponent systems with an amorphous structure, biological objects, etc.

Among the priority analytical tasks, it should be noted:

- Investigation of the content of light impurities with atomic number from $Z = 1$ (hydrogen) to $Z = 12$ (magnesium) in materials in different structural states from liquid to coarse-grained polycrystals.
- Detection of light impurities in metals. This is especially pronounced in metal-hydrogen systems, in which it is possible to reach the limit of detection at a level of $10^{-4} \div 10^{-3}$ mass %.
- Study of modified surfaces. Namely, the control of the distribution of light elements over the depth of the sample, which affects the strength characteristics of materials.
- Elemental and phase analysis of biological objects.

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Застосування ефекту Комптона для вирішення задач фізики конденсованого стану

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Розглянуто перспективи застосування рентгенівських спектральних методів у нових галузях через використання явища розсіювання, як основи для хімічного та фазового аналізу. Теоретично показано, що чутливість методу розсіювання не залежить від структури та якості поверхні зразка і різко зростає із зменшенням атомного номеру домішки, що аналізується. Проаналізовано чутливість методу при дослідженні багатокомпонентних стандартів стехіометричного складу на основі H, Li, B, C, O і F, та порівняно її з чутливістю традиційних аналітичних методів. Розраховано концентраційну чутливість виявлення вмісту легких домішок у металах і наведено експериментальне підтвердження для систем титан-водень та залізо-вуглець. Вперше метод Комптона узагальнено для аналізу багатокомпонентних систем невідомого складу. Для цього, з використанням підходу [13], введено поняття ефективного атомного номеру за властивістю розсіювання. Показано, що залежність ефективного атомного номеру від параметру *x*, що віддзеркалює умови зйомки (кут розсіювання та довжину хвилі первинного випромінювання), однозначно визначає багатокомпонентну сполуку. На підставі аналізу чутливості обґрунтовано діапазон застосування методу розсіювання. З боку малих значень параметру *x*, метод обмежується брегівськими відбиттями, що накладаються на релеєвський пік. При великих значеннях параметру *x*, чутливість методу погіршується через велику розбіжність між інтенсивністю когерентного і некогерентного розсіювання. Наведено приклади вирішення аналітичних завдань, при яких використання рентгенофлуоресцентного та дифракційного аналізу або сильно ускладнене, або взагалі неможливо.

Ключові слова: Відношення інтенсивностей релеєвського та комптонівського розсіювання, Ефективний атомний номер, Легкі елементи, Стехіометричні сполуки.