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Intelligent Precise Goniometric System of Analysis of Spectral Distribution Intensities for Definition of Chemical Composition of Metal-Containing Substances

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The article dedicated to urgent task—definition of chemical composition of metal-containing substances. The new precise intelligent goniometric system, which contains laser goniometer, CMOS image sensor, and artificial neural network, is proposed. This system combines the advantages such as safety for humans and environment, high productivity, usage simplicity, universality, automated processing of the measuring data.

Key words: laser goniometer, chemical composition, spectral distribution, artificial neural network, saturation current, wavelength of light, photocell sensitivity.

Статтю присвячено актуальній проблемі — визначенню хемічного складу металовмісних речовин. На основі аналізи методи спектроскопії, нейромережевих технологій і фізичних принципів роботи фотоелементів запропоновано нову прецизійну інтелектуальну гоніометричну систему на

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основі лазерного гоніометра, CMOS-матриці та штучної нейронної мережі. Система уможливлює проводити аналізу інтенсивностей спектрального розподілу. Вона поєднує такі переваги як безпечність для здоров'я людей і навколишнього середовища, високу продуктивність, простоту використання, універсальність, можливість автоматизованого оброблення вимірювальної інформації.

Ключові слова: лазерний гоніометер, хемічний склад, спектральний розподіл, штучна нейронна мережа, струм наситу, довжина світлової хвилі, чутливість фотоелементів.

Статья посвящена актуальной проблеме — определению химического состава металлосодержащих веществ. На основе анализа метода спектроскопии, нейросетевых технологий и физических принципов работы фотоэлементов предложена новая прецизионная интеллектуальная гониометрическая система на основе лазерного гониометра, CMOS-матрицы и искусственной нейронной сети (ИНС). Система позволяет проводить анализ интенсивностей спектрального распределения. Она объединяет такие преимущества как безопасность для здоровья людей и окружающей среды, высокую производительность, простоту использования, универсальность, возможность автоматизированной обработки измерительной информации. Высокая производительность работы системы достигается за счёт возможности ИНС осуществлять одновременную обработку множества цифровых данных методами параллельной обработки. Безопасность системы обеспечивается за счёт применения принципов лазерной спектроскопии и исключения вредного рентгеновского излучения. Высокая точность системы достигается за счёт использования CCD- и CMOS-матриц с большой разрешающей способностью в качестве чувствительных элементов.

Ключевые слова: лазерный гониометр, химический состав, спектральное распределение, искусственная нейронная сеть, ток насыщения, длина световой волны, чувствительность фотоэлементов.

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1. INTRODUCTION

Determination of chemical composition is urgent production task in case of sorting of the scrap metal, products at the warehouses for incoming control of raw materials in metallurgy, for products' certification, *etc.*

To solve this task nowadays, the special measuring tools based on spectroscopy methods are being used. Spectroscopy is the most important method for analysis of metals chemical composition. In this method, the inspected sample is briefly exposed to a concentrated and sufficiently powerful energy pulse. As a result, the emission spectrum has been formed. This happens due to absorption irregularity of energy by different metallic atoms. Measuring the scattering angle of the emitted radiation allows us to determine the corresponding compounds in metallic materials.

Currently, there are some tools, which allow detecting certain chemical elements in metallic materials by x-ray spectroscopy—x-ray optical instruments and laser spectroscopy—laser optical instruments.

The most common are x-ray instruments, where examined sample exposed to x-ray radiation. Obviously, the systematic x-ray usage is harmful to the health of staff even at low doses [1]. Moreover, x-ray instruments detect chemical elements in limited range. Meanwhile, using of complicated algorithms of data processing increases loss of time on studying and work of instruments. Those disadvantages points on non-expediency of x-ray instruments usage, even in industrial scale.

The use of laser optical instruments is more accurate and is safer than x-rays [2, 3]. In general, laser spectroscopy method has many advantages, comparing to x-ray spectroscopy [4]. First, it is safety and possibility to detect nearly all chemical elements.

Authors in [3] present the results of laser spectroscopy usage for detection of metals in textile dyes. The results of the study revealed the presence of such toxic metals as Cr, Cu, Fe, Ni, and Zn. Moreover, Al, Mg, Ca, and Na have been detected as well. In that research, optical resolution was 0.06 nm, spectral range was 200–720 nm, but it took quite long time.

In [4, 6], authors present the results of detection of heavy metals in soil samples [4] and metals [6] by laser spectroscopy method. Comparison of the given results to the traditional chemical methods demonstrated high accuracy of laser spectroscopy and optical instruments, respectively. In [6], it has been specified that laser spectroscopy is a method, which can provide quantitative and qualitative measurement of the characteristics of irradiated metals. Authors in [6] calculated plasma parameters, which have been given from the sample of brass alloy by pulse of Nd:YAG laser. Unfortunately, authors do not mention the time, which has been taken by system for detection of chemical elements. According to the information provided in the paper, it can be supposed that period was quite long.

In [5], authors describe new approach to measure of chemical composition of the aerosol substance in real time using plasma spectroscopy and a broadband spectrometer with a range of wavelengths of 200–980 nm. The delay of single sensor is 1.3 μs. The disadvantage of the method is impossibility to detect such chemical elements as Cd, Cr, Cu, Mn, Na and Ti. At the same time, the sampling time was 5 min.

In general, there are many different modern methods for determination of chemical composition of metal-containing substances. The analysis on the last one allow to conclude that all of them have different measuring range, accuracy, and speed as well as based on using different mathematical models, methods, and algorithms of data processing, *e.g.*, multidimensional analysis by least squares method [7], multivariate regression in orthogonal Chebyshov polynomials, which are transformed in algebraic polynomials [8] *etc*.

Technical parameters of some wide used means for spectral analysis of metals and alloys are shown in Table 1.

Thus, it can be argued that the problem of qualitative and quantitative determination of chemical elements in metals in real time is still not completely solved. This is due to the fact that modern production in accordance with international quality standards constantly puts ever more stringent requirements for the performance of measuring in-

TABLE 1. Spectrometers and measuring systems, which are based on them.

Model	Main technical and metrological parameters, advantages and disadvantages	Description	Producer
Optical and capacity spectrometer ARL 4460 [9] 	Wave length setting error, nm ±1.5. Spectral range, nm –325–1000. Control system has special software OXSAS. **Advantages:** automated processing of the data. **Disadvantages:** Complex mathematical models and algorithms of data processing.	Analysis of metals and alloys with different base (Fe, Al, Ni, Ti, Cu, Zn, Co, Mg, Pb, Sn, Ag, Au, Pt, Pd)	US, Thermo Fisher Scientific [9]
Capacity spectrometer ‘Iskroline 100’ [10] 	The random relative error, % –0.5–40. Spectral range, nm –174–441. Control system contains PC, controller, and special software compatible to Windows 98/2000/XP/7. **Advantages:** automated processing of the data. **Disadvantages:** quite high random error (40%), unknown value of systematic error, impossibility of real-time data processing, dependency of results on quality of state standard samples, complex mathematical models algorithms of data processing.	Desktop spectrometer for spectral analysis of metals and alloys with different base (Fe, Al, Cu, Zn, Pb, Sn, Sb, Ni, Ti, Co, Mg)	Russia ‘Iskroline’ [10]

Continuation of TABLE 1.

Model	Main technical and metrological parameters, advantages and disadvantages	Description	Producer
Atomic capacity spectrometer 'ISKROLINE 300' [10] 	Relative random error (in dependence on element of mass value), % –0.5–40. Spectral range, nm –174–960. Control system contains PC, controller, and special software Compatible to Windows 98/2000/XP/7. **Advantages:** automated processing of the data. **Disadvantages:** quite high random error (40%), unknown value of systematic error, impossibility of real-time data processing, dependency of results on quality of state standard samples, complex mathematical models algorithms of data processing.	Spectrometer for spectral analysis of metals and alloys with different base (Fe, Al, Cu, Zn, Pb, Sn, Sb, Ni, Ti, Co, Mg) in laboratories	Russia 'Iskroline' [10]
Spectral photometer ULAB 102 [11] 	Wave length setting error, nm ±1.5. Spectral range, nm –325–1000. Control system has special software, which is incompatible to Windows. **Advantages:** automated processing of the data. **Disadvantages:** unknown value of random error, unknown reliability; unknown principles of software operation and algorithms of data processing.	Spectrometer for measuring of the transmission coefficient, optical density of the investigated solid samples and calculating the optical density	China, Ulab [11]

struments. The indicators of the efficiency of measuring systems is safety for humans and environment, accuracy, high productivity, versatility, work in automated mode and real-time mode.

To implement them in the development of new and improved known devices, it can be achieved by using of high-quality optical systems, precision sensors, as well as the state of the art algorithms, methods and procedures for data processing, in particular, using of artificial neural networks (ANN).

It is known that ANN can be successfully used for solving different tasks of processing and analysis of the set of rapidly changing data in real-time mode and in conditions of incompleteness, inconsistency and dynamism of incoming information [12, 13]. Use of ANN is well known in algorithm for evaluation of the angle of knee [14], in the method of prediction of the angle of finger joint [15]. Use of ANN is also well known in the method for evaluation of generator rotation angle and its speed, in particular, for stability analysis and control of transient processes in real-time [16]. It is also known that the system of automated Cobb angle measuring is based on ANN for scoliosis examination [17]. The use of ANN leads to the rise of productivity, reliability and accuracy of work performed.

Purpose of the present work is to suggest precise measuring goniometric system with artificial neural network based on the analysis of physical principles of spectrometry, work of semiconductor photocells and artificial intelligence.

2. DESCRIPTION OF THE PROPOSED SYSTEM

The system is developed on the basis of state of the art research in science and technology in fields of optics, mechanics, electronics, automation, artificial intelligence. It combines such advantages as safety for humans' health and environmental security, high productivity of the analysis, accuracy, wide range of materials, which can be studied, simplicity of use, universality, automated processing of measuring data in real-time.

The structure of intelligent precise goniometric system (IPGS) of analysis of spectral distribution intensities for definition of chemical composition of metal-containing substances is shown in Fig. 1.

The system contains rotation drive *1*, object desk *2*, rotational device, ring laser, optical system *5*, and image sensor *6*, *e.g.*, CMOS sensor for registration of radiation in infrared range or CCD in ultraviolet one, control unit *7*, ANN module *8*, and computer *9*.

Drive *1* mechanically linked to the object desk *2*, which is mounted on the rotational device *3*. Ring laser *4*, optical system *5*, and image sensor *6* are rigidly fixed to the mentioned device. Ring laser *4* and image sensor *6* connected to the control unit *7*. ANN module *8* is interfaced to the computer *9*. One output of the control unit *7* is connected to the input of computer and the other one to the ANN's *8*.

The ring laser *4* is used as a source of a powerful energy pulse, which affects measured object (MO), namely, metal sample, in a short time. MO forms appropriate radiation spectrum (*e.g.*, Fig. 2) with different

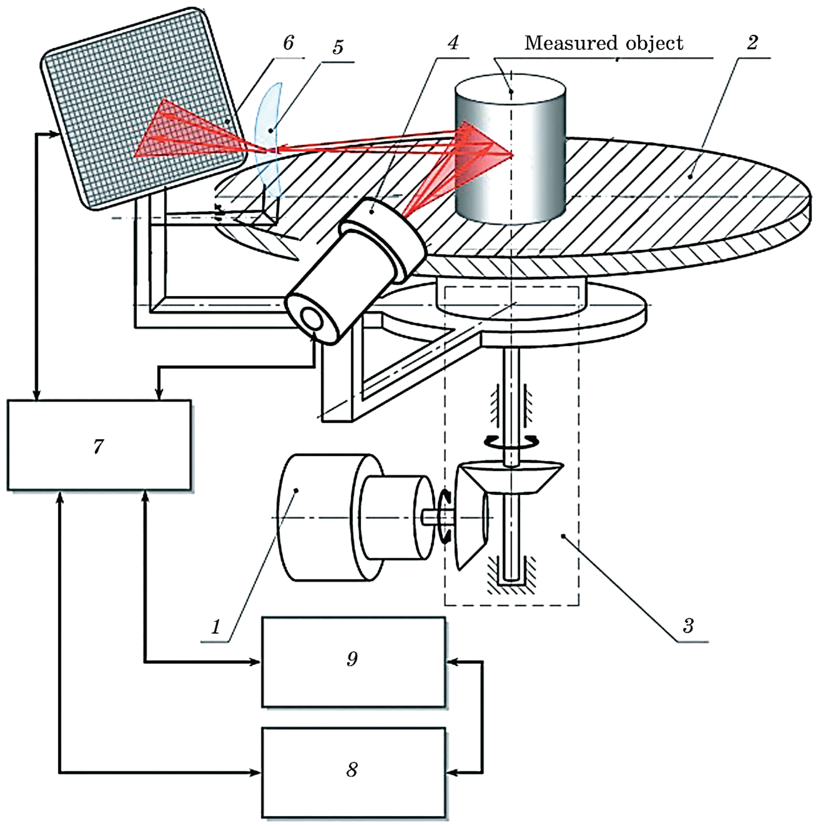

Fig. 1. Block scheme of IPGS of analysis of spectral distribution intensities for definition of chemical composition of metal-containing substances: *1*—rotational drive, *2*—object desk, *3*—rotational device, *4*—ring laser, *5*—optical system, *6*—image sensor, *7*—control unit, *8*—ANN, *9*—computer.

intensities, which depends on its chemical composition.

From [18], it is known that metals strongly reflect radiation in IR range and the range of visible spectrum due to the predominant scattering of light when it interacts with free electrons, whose concentration in metals is 10^{22}–10^{23} cm^{-3}. The electrons emit in scattering of the so-called secondary waves. Absorption of quanta of light directly by electrons is possible only with their simultaneous collisions with photons, impurities of chemical elements, and with each other. It is worth noting, that reflected and absorbed waves are forming not on the surface of metal MO, but in the substance, in so-called near-surface layer, in which the radiation, penetrating into the metal, fades. Optical constants of some metals at room temperature in the visible and infrared spectrum are shown in Table 2.

The luminous flux is projected from the optical system *5* to the im-

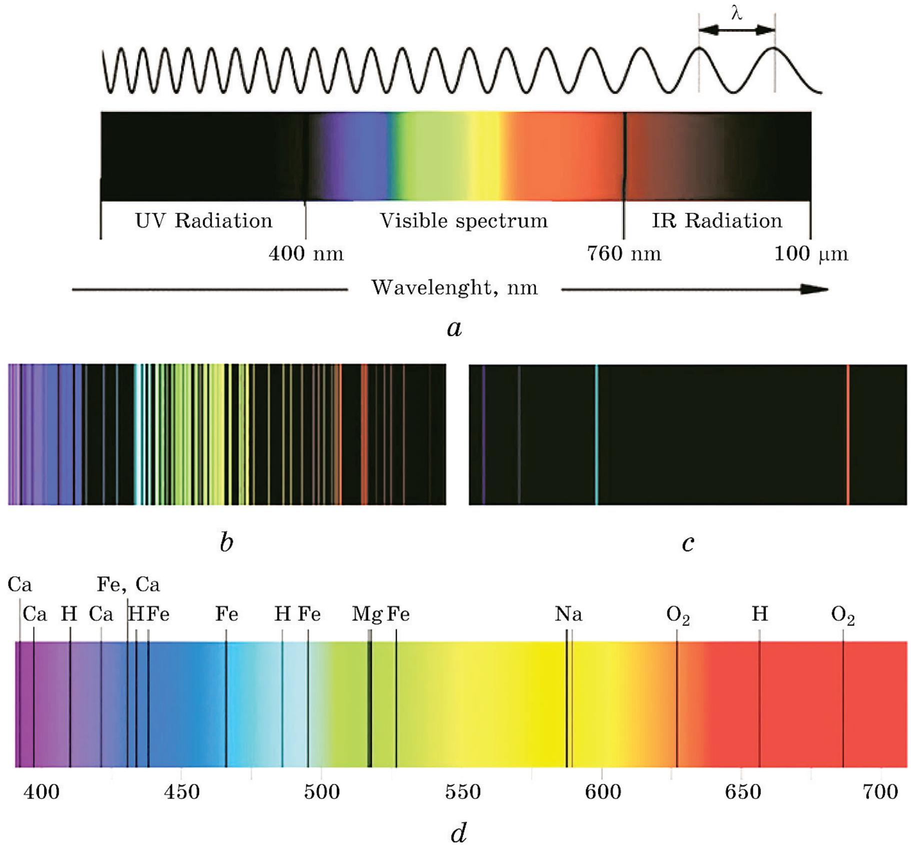

Fig. 2. Electromagnetic spectrum: *a*—range of visible spectrum, *b*—spectrum of Iron, *c*—spectrum of Helium, *d*—excited by the strikes of electrons atoms of various chemical elements.

age sensor *6*, which converts it into an appropriate electrical signal. MO can contain various chemical elements, which absorb energy pulse from the laser *4* with different intensities and form different luminous fluxes. The last ones reflect with different angles and are projected on the different parts of image sensor *6*. It is known [18] that absorption characteristics of metals do not depend on the laser frequency and defined only by their electrical characteristics. The last ones depend on the chemical composition of metals. Electrical signal from image sensor *6* through the control unit *7* are sent to the ANN *8*, which define chemical composition of the studied MO. Computer *9* processes measuring data and presents results in a user-friendly form.

To provide IPGS work in a wide range of visible spectrum, image sensors must meet further requirements: low sensitivity to visible spectrum; high quantum detection efficiency; must have wide local dynamic

TABLE 2. Optical constants of some metals [18].

Metal	$\lambda = 0{,}5$ μm			$\lambda = 5{,}0$ μm		
	Reflective light index, n	Damping coefficient, k_p	Reflection coefficient R, %	Reflective light index, n	Damping coefficient, k_p	Reflection coefficient, R, %
Cu	1,06	2,70	63,2	3,1	32,8	98,9
Ag	0,11	2,94	95,5	2,4	34,2	99,2
Au	0,50	2,04	68,8	3,3	35,2	98,95
Zn	–	–	–	3,8	26,2	97,9
Al	0,50	4,59	91,4	6,7	37,6	98,2
In	–	–	–	9,8	32,2	96,6
Sn	0,78	3,58	80,5	8,5	28,5	96,2
Pb	1,70	3,30	62,6	9,0	24,8	95,0
Ti	2,10	2,82	52,5	3,4	9,4	87,4
Nb	2,13	3,07	56,0	8,0	27,7	96,2
V	2,65	3,33	56,6	6,6	17,5	92,7
Mo	3,15	3,73	59,5	4,25	23,9	97,2
W	3,33	2,96	51,6	3,48	21,2	97,0
Fe	1,46	3,17	63,7	4,2	12,5	90,8
Co	1,56	3,43	65,9	4,3	14,6	92,9
Ni	1,54	3,10	61,6	4,95	18,5	94,8
Pt	1,76	3,59	65,7	7,7	20,2	93,7

range, which is defined as following: maximum value of luminous flux is divided by minimal value of signal, which has been 3% of noise level; must have low sensitivity to background signals and noises.

CCD-, CMOS-image sensors are semiconductor sensors developed on the basis of photocells, *e.g.*, the scheme of CMOS element (complementary metal–oxide–semiconductor) is shown in Fig. 3.

3. PHYSICAL PRINCIPLES OF SENSORS OF THE PROPOSED SYSTEM

The basis of the work of photoelectric semiconductors, that form the basis of the sensors proposed IPGS, particularly CCD and CMOS, is internal photoemission. The last one takes place as follows: when photoelectric semiconductors are exposed to light, they change their inner state. Their conductivity is rising proportionally to the light intensity. The sensitivity S_λ of photocell depends on light wavelength λ and can be defined as follows:

$$S_\lambda = \frac{i(\lambda)}{K\varepsilon r_\lambda \lambda\alpha S}, \quad (1)$$

where S_λ—sensitivity of semiconductor photoelectron element, $i(\lambda)$—

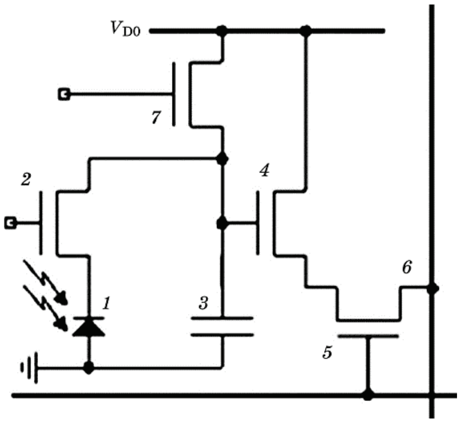

Fig. 3. Equivalent scheme of CMOS element by Micron Technology: *1*—photocell, *2*—gate, 3—capacity, *4*—amplifier, *5*—bus for row changing, *6*—vertical bus, *7*—reset.

saturation current of photocell, K, ε—proportion factors, r_λ—spectral emissivity of the photocell, λ—light wavelength, α—spectral absorption of the material.

Function $f(\lambda)$ of dependence of sensitivity S_λ on light wavelength λ is defined as follows:

$$f(\lambda) = \frac{i(\lambda)}{r_\lambda \lambda}, \tag{2}$$

where $i(\lambda)$—saturation current of photocell, when it is exposed to light with wavelength λ, in accordance with Stoletov's law (or the first law of photoeffect), is expressed by (3):

$$i(\lambda) = \beta S_\lambda \Phi(\lambda), \tag{3}$$

where S_λ—photocell sensitivity on the wavelength λ, $\Phi(\lambda)$—luminous flux, which hits to the photocell, β—proportion factor.

Luminous flux $\Phi(\lambda)$ is a part of light energy $E(\lambda)$, which is emitted by MO, which is exposed to energy pulse of laser (4) with the wavelength λ in range Δλ. We can suppose that:

$$\Phi(\lambda) = KE(\lambda), \tag{4}$$

where K—proportion factor, $E(\lambda)$—light energy, which is emitted by MO and defined by the expression (5):

$$E(\lambda) = r_{\lambda OB} \Delta\lambda S_{OB}, \tag{5}$$

where $r_{\lambda OB}$—spectral emissivity of MO, which is exposed to energy pulse of laser (4) with the wavelength λ in range $\Delta\lambda$ and is defined by the optical system (5) filter bandwidth of IPGS, S_{OB}—MO surface area which is exposed to, $\Delta\lambda$—wavelength range, which is expressed by optical filter bandwidth mentioned above: $\Delta\lambda = \varepsilon\lambda$, where ε—proportion factor.

Spectral emissivity of MO obeys Planck's law, which describes spectral density of electromagnetic radiation emitted by a black body in thermal equilibrium at a given temperature T:

$$U(\omega, T) = \frac{\omega^2}{\pi^2 c^3} \frac{\hbar\omega}{e^{\hbar\omega/(kT)} - 1}, \tag{6}$$

where $\hbar = 1.054 \cdot 10^{-34}$ J·s—Planck constant, $k = 1.38 \cdot 10^{-23}$ J·K^{-1}—Boltzmann constant, $c = 3 \cdot 10^8$ m/s—speed of light in vacuum.

Spectral emissivity of MO $r_{\lambda OB}$ will depend on emissivity $r'_{\lambda OB}$ of chemical elements: $r_{\lambda OB} = f(r'_{\lambda OB})$. Emissivity value of i-th chemical element in accordance to spectral emissivity of black body by Planck's law and equation (8) can be found from the following expression:

$$r'_{\lambda OB} = r_\lambda \alpha_i, \tag{7}$$

where α_i—spectral absorbance capacity of i-th chemical element which is in MO.

Spectral emission of black body by Planck's law is:

$$r_\lambda = 2\pi h c^2 \frac{\lambda^{-5}}{e^{hc/(kT\lambda)} - 1}, \tag{8}$$

where $h = 2\pi\hbar$.

Thus, image sensor forms electric signals in accordance to spectral composition of MO emission, which is caused by chemical elements in its composition.

4. DESCRIPTION OF ARTIFICIAL NEURAL NETWORK

ANN *8* allows automated detection of some chemical elements contained in MO by digital signals from image sensor *6*. ANN can be either neural processor or, *e.g.*, neural simulator with customizable structure of neurons by one of the known models (*e.g.*, multilayer perceptron). Mathematical model of neuron is shown below:

$$NET = \sum_{i=1}^{P} w_i x_i, \; OUT = F(NET - \theta), \tag{9}$$

where NET—weighted sum of input signals, w_i—synapsis weight ($i = 0, 1, 2, \ldots, p$), x_i—component of input vector signal ($i = 0, 1, 2, \ldots,$

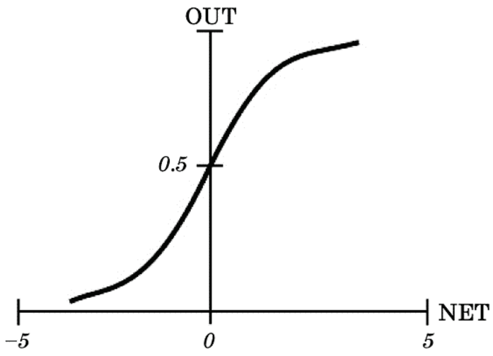

Fig. 4. Logistic activation function (Fermi or sigmoid).

p), p—number of neuron inputs, θ—value of shift, OUT—output signal of neuron, F—non-linear transducer that realize activation function $OUT = f(NET)$ (Fig. 4):

$$OUT = \frac{1}{1 + e^{-NET}}.$$

Block scheme of artificial neuron is shown on Fig. 5.

ANN is trained by supervised learning with backpropagation method to recognize chemical elements in metals. It assumes that ANN is pre-trained by using of empirical given values of intensities of spectral lines and main physical laws of chemical elements in metals to detect their into different metal samples. ANN *8* by the appropriate algorithm processes digital signals from CMOS sensor. The set of saturation current of photocell are sent to the input of ANN. These currents occur due to irradiation MO with light with wavelengths λ_i: $\{i_i(\lambda_i) \mid i \in \{$C, P, S, Mn, Si, Cr, Ni, Cu, Nb, N, Al, Ti, V, Mo, W, Co, B, Fe$\}\}$, where C, P, S, ..., Fe—are the symbols of some elements which can

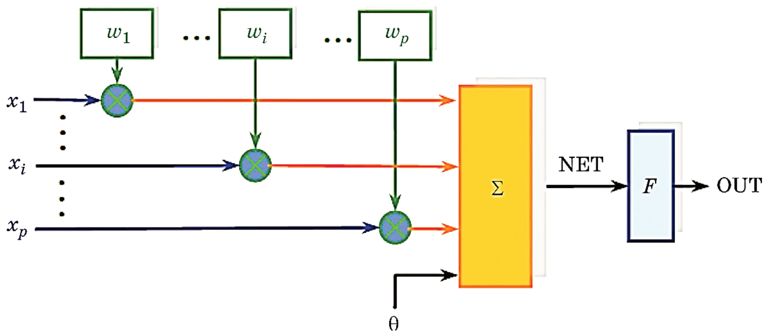

Fig. 5. Block scheme of artificial neuron.

be in MO. The set of saturation currents, as required by ANN, form input layer $X = \{x_j \mid j = \overline{1, J}\}$, which is sent to its (ANN) input (Fig. 6 and 7). Dimension of input layer and number of neurons at ANN's input, which is used to receive input data from CMOS, has been conditioned by image sensor resolution.

ANN forms digital signal, which reflects chemical composition of studied MO in form of digital signal vector Y: $Y = \{y_m \mid m = \overline{1, M}\}$, where M—number of chemical elements, which can be detected. Maximal value y_m at m-th output of ANN means that appropriate chemical element exists in MO contain (Fig. 6 and 7).

ANN's signal is sent to the computer *9*, which processes it and presents a result in a user-friendly form.

Block scheme of the ANN *8* for automated detection of chemical elements in metals is shown in Fig. 6. ANN is built as multilayer perceptron with 3-layer structure; numbers of neurons in each layer are caused by the task.

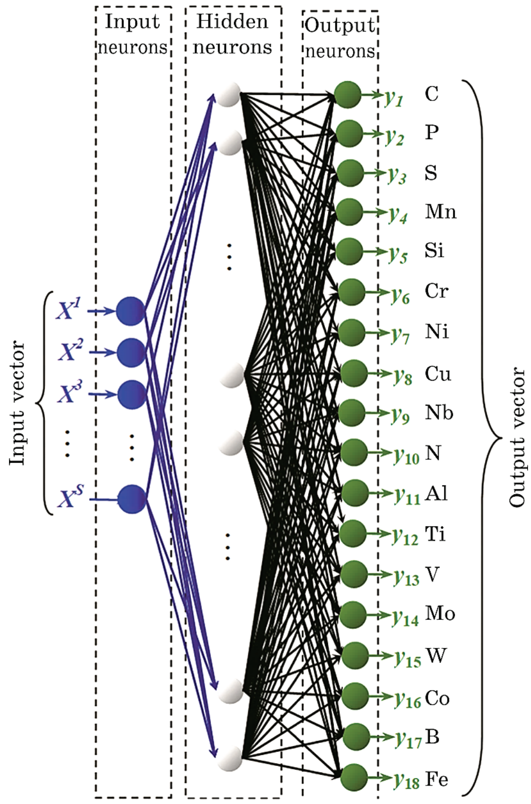

Fig. 6. Scheme of ANN for automated detection of chemical elements in metals.

Number of neurons on ANN's output is caused by the structure of output vector Y. The decision about presence of one or another chemical element in metal is taken by so-called answer interpreter 'Winner-

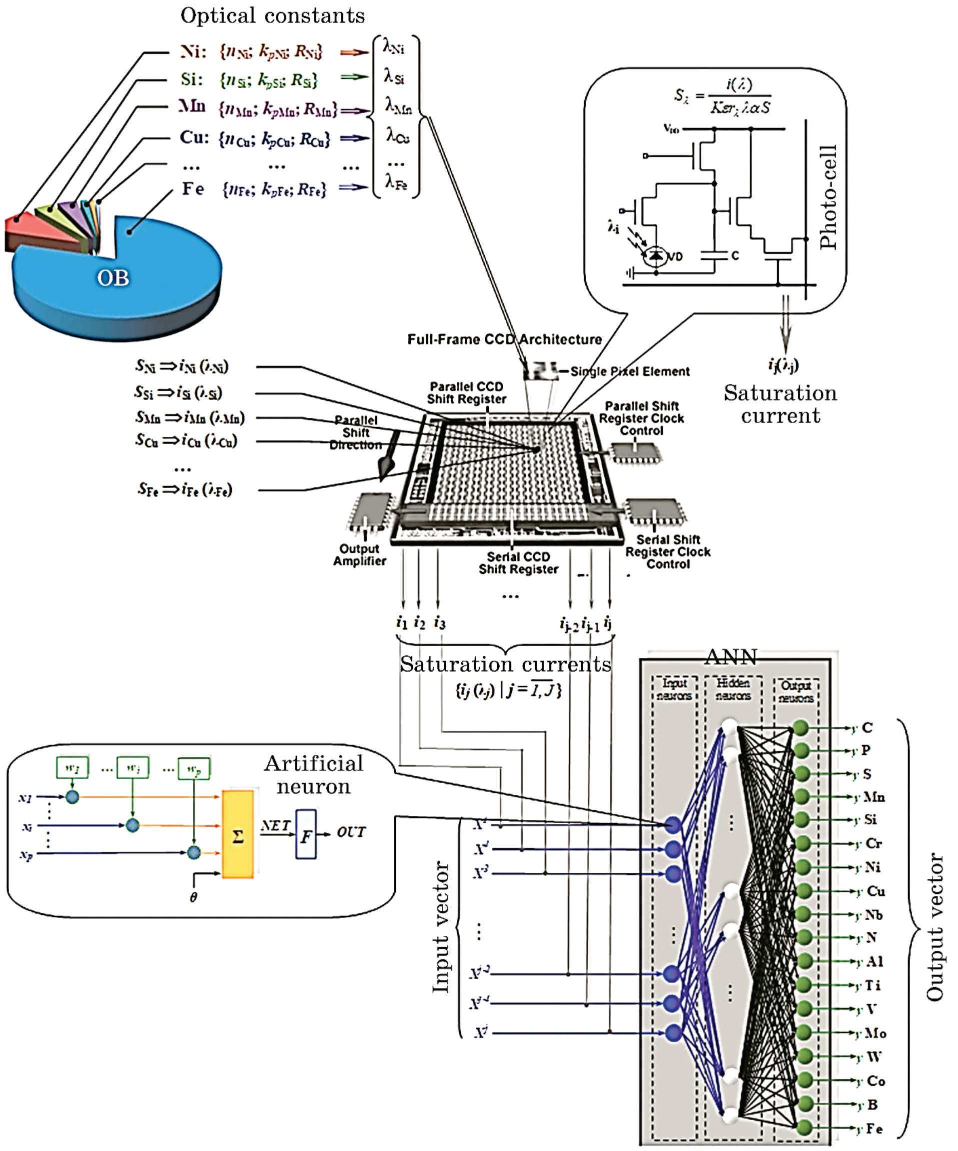

Fig. 7. Scheme of ANN's interaction with the image sensor of the proposed Intelligent Precise Goniometric System in automated analysis of spectral distribution intensities for definition of chemical composition of metal-containing substances.

take-all'. According to the last one, number of output signals corresponds to the number of choice of answers. Number of the answer corresponds to the number of neuron that has maximum output signal. Appropriate inputs of ANN will receive maximal values of signals, which mean that appropriate chemical elements are in metal MO.

So, the structure of output vector can be presented as Table 2. It must be noted that the number of components of output vector can be increase in proportion to increasing of image sensor sensitivity. In accordance to that, the number of ANN's outputs can be increased. This allows increasing the range of the elements detected.

Hidden layer provides intermediate data processing in the way that linear distributed set be sent to the output layer of neurons. The dimension of hidden layers is empirically defined following to the results of ANN's learning. Error value is the criteria under which ANN training is cancelled; this value must be less than 0.05 that equals to 5%.

Figure 7 shows the scheme of ANN's interaction with the image sensor in automated analysis of spectral distribution intensities for definition of chemical composition of metal-containing substances.

5. CONCLUSIONS

1. The time of data processing is significantly decreasing due to the ANN's feature of parallel processing of data sets. This causes rise in productivity of the system as a whole.
2. The system provides safety for humans and environment with the use of laser radiation instead of harmful x-rays.
3. High accuracy of the system is achieved by using either high sensitive CCD or CMOS elements as the image sensor, which perceives spectral radiation with high resolution.
4. All mentioned above allows to state that proposed system has further advantages: the system has high productivity and allows brief analysing because of the use of ANN which provides parallel processing of the set of digital data; the system is harmless to humans' health and environment due to use laser source instead of x-ray one; universality because of the use of CCD or CMOS elements, which allow expanding the range of chemical elements detected.

In general, we can assume that the proposed system is a modern and promising development.

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