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ORIGINAL RESEARCH PAPER

METHODS OF ANALYSIS AND CLASSIFICATION OF THE COMPONENTS OF GRAIN MIXTURES BASED ON MEASURING THE REFLECTION AND TRANSMISSION SPECTRA

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Abstract: The paper considers methods of classification of grain mixture components based on spectral analysis in visible and near-infrared wavelength ranges using various measurement approaches - reflection, transmission and combined spectrum methods. It also describes the experimental measuring units used and suggests the prototype of a multispectral grain mixture analyzer. The results of the spectral measurement were processed using neural network based classification algorithms. The probabilities of incorrect recognition for various numbers of spectral parts and combinations of spectral methods were estimated. The paper demonstrates that combined usage of two spectral analysis methods leads to higher classification accuracy and allows for reducing the number of the analyzed spectral parts. A detailed description of the proposed measurement device for high-performance real-time multispectral analysis of the components of grain mixtures is given.

Keywords: *grain mixtures, neural networks, pattern recognition, seed quality, spectral analysis*

INTRODUCTION

For correct classification of grain mixture components required for seed quality analysis, the latest achievements in computer science, electronics, and high-performance recorders and digital processors of signals and images can be used. One of the most productive ways of solving this problem is to use spectral analysis methods for obtaining the necessary data, and the latest machine learning methods for further processing of this data.

Variations in seed quality caused by the cultivation technology, soil and climate conditions, hereditary and mutagenic factors, etc. often result in lower yields. It is, therefore, important to keep the seeds with high purity of variety. For example, the purity of variety for wheat seeds [1] of original or elite category should be greater than 99.7 %, for the reproduction seeds category it is 98 %, and for the commercial reproduction seeds - 95 %. Such parameters as seed dockage, presence of diseases, pests and defective seeds, are also carefully analyzed in biological crop farming industry.

The seed quality is determined not only by the purity of variety, but also by such parameters as the seed color, vitreousity, presence of foreign materials and diseased grains, as well as by such biologically significant indicators as the concentration of proteins, gluten, fats, carbohydrates, and the humidity level. Each variety has its own unique biomolecular structure and content. The ratio between biologically significant indicators, such as total protein, starch, fat content or concentration, etc., can be used to identify the seed's variety [2].

To determine the seed quality, chemical methods are usually applied. One of the most effective methods is the molecular marker method based on studying polymorphism of proteins (reserve proteins in the first place) and nuclear acids of the seeds. Using reserve proteins as molecular markers resulted in significant advances in seed identification, as well as in registering the varieties crucial for seed production and control [3 – 5]. To analyze the biological value and viability of the seeds, standard chemical methods are usually used [6 – 7].

These methods have proved to be effective in the field of selection and seed production, but their application for analyzing large amounts of seeds is limited. The main reason is that they are very time-consuming and require expensive chemical equipment, various reagents, and specially trained personnel. Furthermore, these methods are destructive.

An alternative way is based on using optical spectroscopy methods, which are now applied widely in the sphere of agriculture and food quality control. Furthermore, as demonstrated in [8 – 12], these methods can be used to produce real-time sensors for high-performance optical grain sorters designed for real-time sorting of large amounts of seeds.

A long history of studies has shown that it is quite reasonable to perform spectral analysis of complex samples in visible and near-infrared wavelength ranges, studying, for example, oscillations of the O-H, C-H, C-O and N-H bonds and thus estimating the biological value of the elements of the grain mixture. This method is not destructive, and at the same time, it is relatively inexpensive. There are many papers concerning the near-infrared spectroscopy methods used for estimating the quality of the grains, or detecting the diseased or defective grains [13 – 22]. For further computer processing of the spectral measurements, various machine-learning algorithms were used: partial least squares discriminant analysis, soft independent modeling of class analogy, *K*-nearest neighbors, and least squares support vector machines.

The fact that various near-infrared rapid analyzers (NIR analyzers [23 – 27]) are now available on the market, demonstrates that the success reached in solving the problem of estimating the biological value is quite remarkable. These analyzers are widely used in grain, flour-milling, food and feed industries. One of the most important tendencies of their further development is that universal and relatively cheap equipment with higher performance and accuracy is designed all the time.

The available rapid analyzers usually apply only one spectral analysis method, for example, analysis of reflection, transmission, absorption, or photoluminescence spectrum. We believe that combined usage of several spectral methods can significantly improve the biological value analysis and extent the sphere of application of rapid analyzers. Furthermore, the available analyzers perform spectral analysis of reflected or transmitted light on multiple grains. This is acceptable in food or feed industries, but seed industry needs each object to be analyzed separately.

Therefore, it is important to study various spectral methods of estimating seed quality and purity of variety, as well as to consider the effectiveness of their combined usage and studying classification algorithms for analyzers of combined type.

MATERIALS AND METHODS

Subject of the research and spectrum measurement techniques

As the subject of the research, we selected three varieties of triticale: two winter varieties “Doktrina 110” and “Gorka”, and a spring variety “Ukro”. The seeds were cultivated, and kindly provided to the authors by Dokuchaev Agricultural Research Institute.

Triticale is a hybrid of wheat and rye [28]. It is a valuable crop containing a lot of protein (gliadin) and rich in glutamic acid and proline [29]. The average content of protein is 1 - 1.5 % higher compared to wheat and 3 - 4 % higher compared to rye. It has the same content of gluten as wheat, but the gluten’s quality is lower. We used molecular markers to specify reference groups of each variety by registering the electrophoretic spectra of the reserve proteins. It should be noted, that the seeds of each variety are similar in shape and color.

To identify the seeds’ variety, reflection and transmission spectroscopy methods in visible and near-infrared (up to 1000 nm) wavelength ranges were used. Reflection and transmission spectra in visible and near-infrared light were measured using experimental measuring units based on optical-fiber spectrometer USB4000-VIS-NIR.

The reflection spectra were measured using the experimental unit shown in Figure 1. Light from the HL-2000 (Ocean Optics) light source 1 passes through the light guide 2 into the ISP-50-8-R-GT (Ocean Optics) integrating sphere 3 at an angle of 8°. Numerical aperture (NA) of the optical fiber is 0.22. The light reflected from the sample 4 at an angle of 90° emerges from the integrating sphere and passes through the light guide 5 to the spectrometer 6, connected to a computer 7. A WS-1 reflection standard served as the source of reference signal.

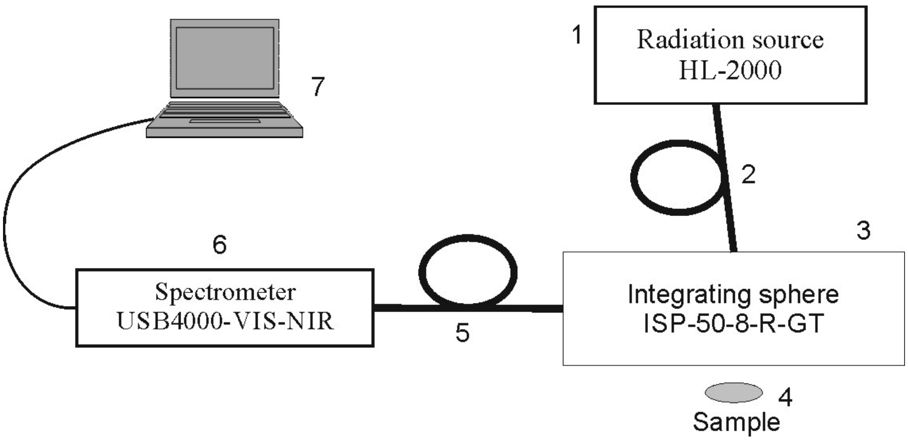

Figure 1. *Experimental unit for measuring the reflection spectra*

Collimated transmission spectra were measured using the experimental unit shown in Figure 2. Light coming from the HL-2000 (Ocean Optics) light source 1 passes through the light guide 2 to the collimator 3. Numerical aperture of the optical fiber is 0.22. Collimator 3 contains an aspherical lens element with NA = 0.51. The quasi-collimated light beam is then directed to the sample 4. The light beam diameter (around 1.5 mm) is about one-half of the average thickness of the analyzed grains (around 3 mm). Collimator 5 collects the transmitted light and passes it through the output light guide 6 (NA = 0.5) to the spectrometer 7, connected to the computer 8. Collimator 5 contains an aspherical lens element with NA = 0.51. The distance between collimator 5 and the grain is around 3 mm. Specialized triaxial supports (Thorlabs) are used to arrange the optical axes of the collimators on the same line with the sample. An additional iris diaphragm can be placed after the collimator 3 to increase the dynamic range of the device.

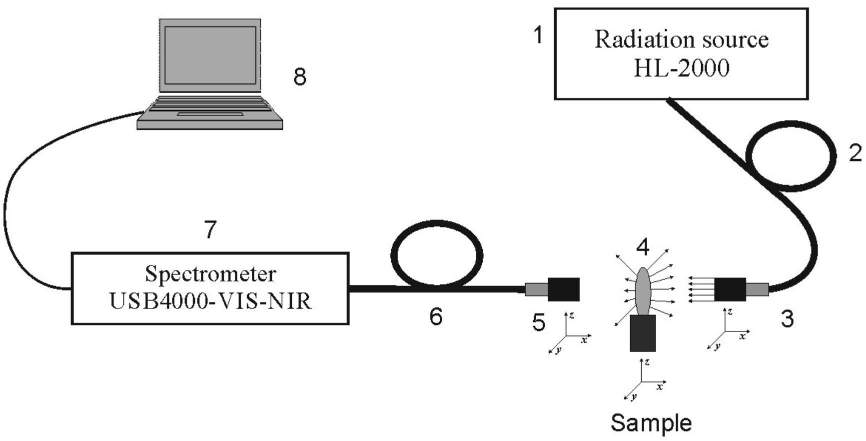

Figure 2. *Experimental unit for obtaining the transmission spectra*

Considering that even seeds of the same class can be quite heterogeneous, we selected 248 seeds of each class at random. For each sample, reflection and transmission spectra were measured. It should also be noted, that for the consistency of the analysis, the seeds used were practically of the same thickness. Possible thickness fluctuations were insufficient compared to the overall thickness.

Spectral data processing methods

Similar research [8 – 10] has already studied various machine learning methods, particularly artificial neural networks (ANN) and support vector machines. Considering that neural networks method has demonstrated better results, in this paper we will focus on the neural networks based learning methods.

To solve the problem of recognizing the objects of grain mixtures, we used a neural network of the MLP (multilayer perceptron) class. Two layers of neurons were used in the network, one of which is hidden with a sigmoid activation function and the other is the output with a linear activation function. The number of input contacts n corresponds to the number of recognition characteristics employed, which were determined basing on the components of the reflection or transmission spectra obtained in the experimental part. The number of neurons in the output layer m_2 corresponds to the number of the seed varieties ($m_2 = 3$), where values “1” and “0” mean that the seed belongs or does not belong to the corresponding variety respectively. The number of neurons in the hidden layer m_1 was selected from the range of values $n \le m_1 \le 2n+1$. The network was created and tested using MATLAB environment. Levenberg-Marquardt algorithm was used for training.

To ensure the invariance of the initial data (the measured reflection and transmission spectra) processing, it was first normalized using MATLAB function mapstd, which processes the matrix of measured values of the spectral components by mapping each component’s means to 0 and deviations to 1.

The initial measurement data contained 2256 spectral components for each measured reflection or transmission spectrum, but such a big number of spectral components is not practical for the problem under consideration. To reduce the dimensions of the initial data to n spectral parts, they were thinned out by averaging Δ neighboring spectral parts for each spectral component:

$$\tilde{s}'_{i,j} = \sum_{t=i}^{i+\Delta-1} s_{t,j} \Big/ \Delta,\ i = \overline{1,N}\ ,\ j = \overline{1,L}\ ,\ \Delta \ge floor\left(\frac{N}{n}\right) \tag{1}$$

where: s' is the matrix of measured values of the spectral components, N is the number of the spectral components, L is the number of the measurements performed, $n < N$ is the total number of spectral parts and $floor\left(\frac{N}{n}\right)$ is the operation of rounding down. After that, the rows of the matrix $\tilde{s}'$ were “subsampled” to get a matrix of averaged spectral components $\tilde{s}$ with dimensions $n \times L$:

$$\tilde{s}_{k,j} = \tilde{s}'_{ind,j}\ ,\ k = \overline{1,n}\ ,\ j = \overline{1,L}\ ,\ ind = (k-1) * floor\left(\frac{N}{n}\right) + 1 \tag{2}$$

To evaluate the classification effectiveness, measurements for 248 samples of each class were made using the experimental measuring units, so the total of $L = 746$ reflection and transmission spectra were measured. The conventional ways of separating data into training and testing sets at a ratio of 2:1 or 1:1 are not suitable for small amounts of data because the testing and training sets are not large enough for proper performance evaluation, so we used cross-validation for testing. Cross-validation presumes selecting one sample from the initial dataset as a testing sample and using the other samples as training samples. This operation repeats several times for different samples and the resulting performance estimate is calculated by averaging the results. The estimates of this kind can be used to find suitable parameters for the algorithm. In case of two object classes the estimates of error probabilities $\tilde{\alpha}(X^L)$, $\tilde{\beta}(X^L)$ can be calculated using the following expressions:

$$\tilde{\alpha}(X^L) = \frac{1}{L_1}\sum_{k=1}^{L_1}\tilde{\alpha}_k(X_k^{L_1-1}, X^{L_2}),\ \tilde{\beta}(X^L) = \frac{1}{L_2}\sum_{k=1}^{L_2}\tilde{\beta}_k(X^{L_1}, X_k^{L_2-1}) \quad (3)$$

where: $\tilde{\alpha}_k(X_k^{L_1-1}, X^{L_2})$ is a type I error indicator taking a value of 0 or 1 when the algorithm, trained on the samples $X_k^{L_1-1}, X^{L_2}$ (all samples except $x^{(1,k)}$), is tested on the sample $x^{(1,k)}$; $\tilde{\beta}_k(X^{L_1}, X_k^{L_2-1})$ is a type II error indicator taking a value of 0 or 1 when the algorithm, trained on the samples $X^{L_1}, X_k^{L_2-1}$ (all samples except $x^{(2,k)}$), is tested on the sample $x^{(2,k)}$.

RESULTS AND DISCUSSION

Results of the spectral analysis

Figure 3 shows the reflection spectra of each class of the samples in visible and near-infrared regions averaged over 248. It demonstrates that reflection spectra of all triticale varieties are very close in visible region and are of similar shape. However, in the near-infrared region there is a slight difference between the spectrum curves.

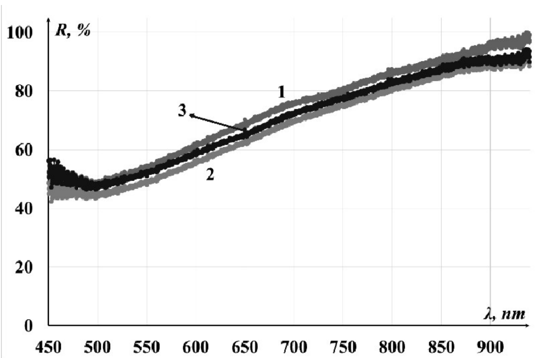

Figure 3. *Average reflection spectra of "Ukro" (curve 1), "Doktrina 110" (curve 2) and "Gorka" (curve 3) triticale seeds*

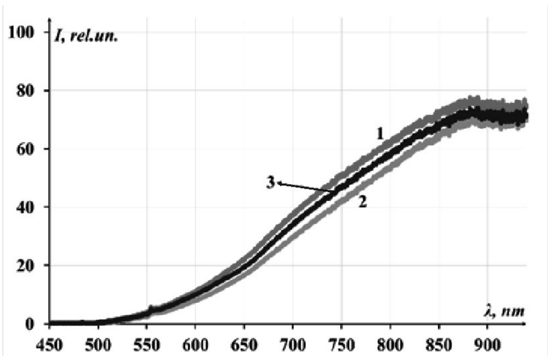

Figure 4. *Average transmission spectra of "Ukro" (curve 1), "Doktrina 110" (curve 2) and "Gorka" (curve 3) triticale seeds*

Figure 4 shows the averaged collimated transmission spectra of each class of the samples. It demonstrates maximum transmission in the near-infrared region and maximum absorption in the region from 450 to 550 nm for all triticale varieties. The difference between the transmission spectra curves is more noticeable compared to the reflection ones. The spectral curve of "Ukro" seeds lies below the "Gorka" curve, and the "Doktrina 110" seeds have the highest transmission factor. The discovered difference between the spectra curves is caused by multicomponent chemical composition of the seeds.

Visual analysis of the results shows that spectral classification of triticale seeds is a difficult task. However, seed classification effectiveness can be increased by combining various spectral methods. Apparently, combined usage of transmission and reflection spectroscopy methods may reduce the classification error probability.

Classification based on single spectral methods

Figure 5 shows the probabilities of incorrect recognition of the triticale seeds variety depending on the number of the spectral parts analyzed. It is obvious that if the number of the spectral parts used for training increases, the error probability decreases significantly. When the threshold $n = 10$ is exceeded, the probability of error becomes sufficiently low and is not reduced when increasing n further. Hence, we can conclude that a measurement unit can be constructed using simpler sensors that register only a few spectral parts. It can be crucial for designing high-performance video spectrum analyzers capable of operating in real-time mode.

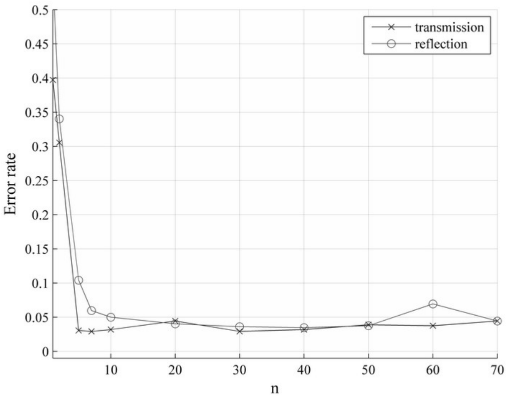

Figure 5. *Probabilities of incorrect recognition of the triticale seeds variety depending on the number of the analyzed spectral parts*

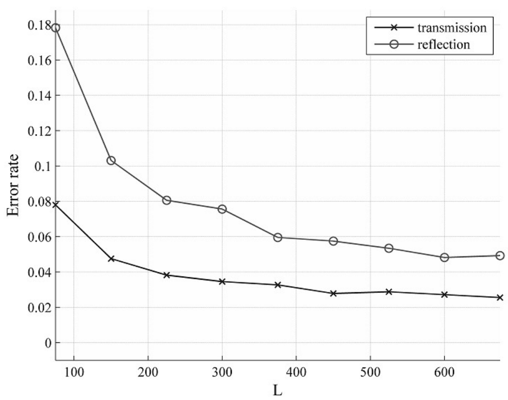

Figure 6. *Probabilities of incorrect recognition of the triticale seeds variety depending on the training set size* L *for* $n = 10$ *analyzed spectral parts*

Furthermore, we studied the dependency between the training set size and the classifier performance to ensure that the dataset used is large enough to provide reliable results. For each training set size (from 75 to 675 samples), 100 tests were performed using bootstrapping: training samples for each test were selected at random from the initial dataset and the remaining samples were used for testing. The aggregated result for each dataset size was calculated by averaging the results for each test. Figure 6 shows the probabilities of incorrect recognition of the triticale seeds variety depending on the training set size.

Figure 6 demonstrates that when the training set size $L = 450$ is exceeded, the probability of error is not reduced significantly with the increased size of the training set, and converges to the fixed value.

Combined use of spectral methods

To increase the classification accuracy, we propose a combined use of several spectral analysis methods. In this case, the input of the neural network contains n measured spectral components for reflection and transmission spectra ($2n$ components in total). Figure 7 shows that combined use of spectral analysis methods provides noticeably higher classification accuracy compared to using a single method even when $n = 2$ spectral parts are analyzed. The error rate for transmission and reflection spectra when used separately is 29 % and 35 % respectively, but for their combination it is only about 20 %. The results for $n = 10$ spectral parts are similar.

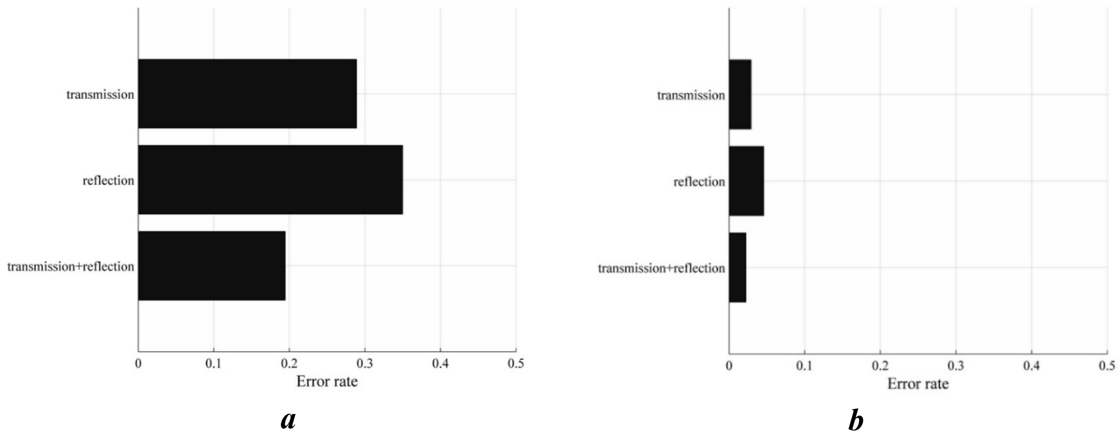

Figure 7. *Probabilities of incorrect recognition of the triticale seeds variety for single and combined spectral methods for* $n = 2$ *(Figure 7a) and* $n = 10$ *(Figure 7b) analyzed spectral parts for each spectrum*

This demonstrates the need for analyzers capable of measuring both reflected and transmitted light. Moreover, solving seed industry problems and purity of variety control require each component of the grain mixture to be analyzed separately and in real-time mode. Obviously, the conventional NIR analyzers cannot satisfy these requirements, because they perform an averaged spectral analysis of multiple seeds using only one spectral method and show a very low performance. To solve that problem we suggest to design a multispectral analyzer capable of performing real-time analysis of the components of grain mixtures and other biologic objects [11 – 12]. The work speed of such an analyzer should be restricted only by the speed of processing the multispectral measurement results.

Laser video spectrum analyzer

The problem of seed classification and sorting can be solved using the device proposed in this paper - a laser video spectrum analyzer. The analyzer can measure reflected and transmitted laser light for four spectral parts at the same time. By changing the type of the line sensor, visible or near-infrared region analysis can be performed. The choice of the sensor depends on the specific task. The device can also recognize and classify objects basing on their color, size, shape and other characteristics available for computer vision. Figure 8 presents a scheme of the video spectrum analyzer.

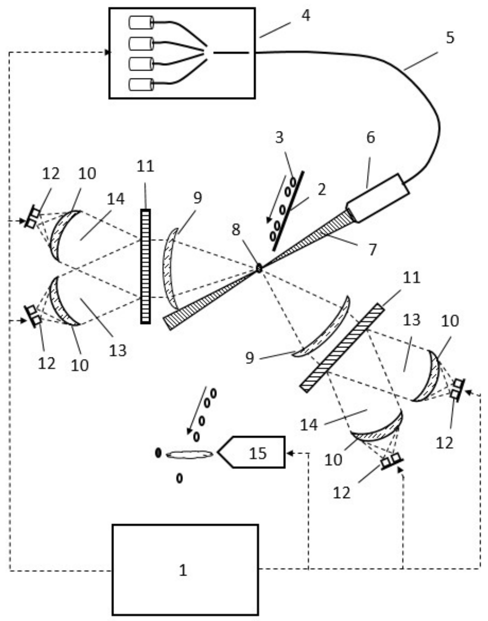

Figure 8. *Optical scheme of the laser video spectrum analyzer*
1 - image capture and processing device, 2 - slope chute, 3 - objects being analyzed, 4 - fiber optic laser light combiner, 5 - fiber optic light guide, 6 - system of cylindrical lenses for spatial distribution of the beam 7 as line 8 in the image capture area, 9 - collimating lenses, 10 - camera lenses, 11 - diffraction grating, 12 - monochrome line sensors grouped in +1 and -1 orders of diffraction 13 and 14, 15 - defective objects removal device

The analyzed objects moving down the chute in a single layer are lighted by laser light of various spectral composition having linear scan focused on the image capture plane. A custom fiber optic device is used to combine two or more laser light sources [12]. The distinctive feature of the analyzer is that it captures digital images of the objects moving at high speed using video camera with monochrome light sensors without light filters. Each pixel of the image has a full set of the laser illumination spectra.
Single line light beam with a specter composed by multiple laser light sources makes the analyzer behave like a spectrometer. Linear light beam plays a role of the entrance slit of the spectrometer. Reflected and transmitted light passes through the collimating lenses and, exiting the phase diffraction grating, is splat into 0, -1 and +1 diffraction orders. The first orders contain all spectral components of the laser sources. The angles between them depend on the wavelengths of the lasers and the diffraction grating constant. The image and line sensors should be aligned on the camera lenses' focal plane in one of the diffraction orders.
The seed feed rate for the proposed analyzer should be determined taking into account the duration of the multispectral analysis. The laser video spectrum analyzer operates in the following way. The seeds that should be separated are fed to a seed transporter that ends with the slope chute 2 forming a monolayer and ensuring a proper feed rate. The seeds are then transferred to the laser lighting and image capture area 8. Fiber optic light combiner 4 controlled by the device 1 produces light at the end of the fiber 5. The light passes to the system of lenses 6 that transforms the light beam into a single line in the

plane of image capture 8. The device 4 combines the light beams of four lasers within a single optical fiber. We should point out, that illumination along the scan line of the laser beam in the area 8 is non-uniform, which is caused by the angular distribution of the light beam, but it could be compensated for by the device 1 at the image synthesis stage. Device 1 controls the video sensors of both the first and second capture devices' cameras synchronously. The collimating lens 9 transforms the angular spectrum of the image of linear area 8 into parallel beams of monospectral components. This is necessary for the diffraction grating 11 to operate properly. Fraunhofer diffraction at the grating 11 is localized on the focal plane of the camera lenses 10 as monospectral images of area 8 at the monochrome sensors 12 in the corresponding diffraction orders 13 and 14. The analog data from the sensors' outputs is transformed into a binary code, and the video processor of the device 1 synthetizes an image of the object 3 in the corresponding spectral regions of the laser light. The software of the device 1 analyzes these monospectral images and decides whether the image meets the selected criteria. If the analyzer detects a substandard object, its location and the time of its arrival to the removal area are registered. The defective object removal device, which is typically a line of pneumatic ejectors controlled by the image processing system 1, removes the defective objects with compressed air and places them in a special tank.

CONCLUSION

Analysis of the results obtained allows for the conclusion, that the proposed spectrum measurement methods combined with neural network based classification algorithms, may provide sufficiently higher seed classification accuracy. Furthermore, the classification accuracy is high enough even when a small number of spectral parts are analyzed, and when the threshold is exceeded, the accuracy almost does not depend on this number. Combined use of spectral methods helps to increase the classification accuracy when small or medium amount of spectral parts are analyzed. Hence, we can conclude that a measurement device for high-performance real-time multispectral analysis can include simpler sensors as compared to the spectrometers we used for the experimental units.

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