

LASER-INDUCED BREAKDOWN SPECTRAL SEPARATION METHOD FOR BAUXITE BASED ON CONVOLUTIONAL NEURAL NETWORK**

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Aluminum alloys are irreplaceable in key lightweight components of automobiles, aircraft, aerospace vehicles, and ships. The main raw material of aluminum alloys is bauxite, and so the high-precision sorting and identification of bauxite is very important in guaranteeing the performance of aluminum alloys. This article describes a convolutional neural network (CNN) structure that, combined with principal component analysis-assisted laser-induced breakdown spectroscopy, can identify different types of bauxite samples. First, the data collected by a spectrometer are normalized to eliminate the influence of different dimensions on the excitation intensities of each spectral line. The feature dimensionality of the normalized samples is then reduced through principal component analysis. The features of the input data are extracted multiple times through convolution and pooling operations in the CNN. Experimental results show that the classification accuracy under a single convolution and pooling structure reaches 97.4%, whereas that under multiple convolution and pooling structures can reach 99.6%. To evaluate the performance of the proposed model, models based on *k*-nearest neighbors, random forest, support vector machine, and full-spectrum feature inputs are constructed. The results show that CNNs have great potential in the field of bauxite identification and classification, and provide a reliable data processing method that enables laser-induced breakdown spectroscopy to classify materials with similar chemical properties.

Keywords: laser-induced breakdown spectroscopy, convolutional neural network, principal component analysis, bauxite.

ИДЕНТИФИКАЦИЯ РАЗЛИЧНЫХ ТИПОВ БОКСИТОВ НА ОСНОВЕ ЛАЗЕРНО-ИСКРОВОЙ ЭМИССИОННОЙ СПЕКТРОСКОПИИ И СВЕРТОЧНОЙ НЕЙРОННОЙ СЕТИ

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Для идентификации различных типов бокситов предложена структура сверточной нейронной сети (CNN) в сочетании с лазерно-искровой эмиссионной спектроскопией методом анализа главных компонент. Полученные на спектрометре данные нормализуются для исключения влияния разных размерностей на интенсивности возбуждения каждой спектральной линии. Размерность признаков нормализованных выборок уменьшается с помощью анализа главных компонент. Входные данные получают с помощью операций свертки и объединения в CNN. Точность классификации при одной свертке и объединении 97.4%, при множественных свертках и объединениях 99.6%. Для оценки про-

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изводительности предложенной модели построены модели, основанные на методах k -ближайших соседей, случайного леса, опорных векторов и входных характеристиках полного спектра. Показано, что CNN обладают большим потенциалом в области идентификации и классификации бокситов и обеспечивают надежный метод обработки данных, который позволяет классифицировать материалы со схожими химическими свойствами с использованием лазерно-искровой эмиссионной спектроскопии.

Ключевые слова: лазерно-искровая эмиссионная спектроскопия, сверточная нейронная сеть, анализ главных компонент, боксит.

Introduction. Aluminum alloy materials are irreplaceable in several key lightweight components in the fields of automobiles, aircraft, aerospace, and shipping. The main raw material of aluminum alloys is bauxite. The content ratio of various chemical components in bauxite and the purity of alumina directly affect the beneficiation and smelting of bauxite and the use of aluminum. Therefore, the high-precision sorting of bauxite is very important in ensuring the performance of aluminum alloys.

Laser-induced breakdown spectroscopy (LIBS) technology has developed rapidly in the past two decades. It is widely used in the analysis of samples of various physical forms because it offers fast analysis speed with no need for sample pretreatment. By analyzing the LIBS signal intensity, the absolute concentration of multiple elements can be measured at the same time. LIBS technology is widely used in material detection [1–3], environmental monitoring [4], gas composition analysis [5], and other fields.

At present, various statistical methods, machine learning techniques, and deep learning algorithms are combined with LIBS for classification, clustering, and regression. Xu et al. will combine convolutional neural network (CNN) with laser-induced breakdown spectroscopy (LIBS) for soil analysis, whereas Banu et al. [7] applied principal component analysis (PCA) and partial least-squares regression to classify meat and measure its adulteration rate. Li et al. [8] used the preselected spectral line and traversal combined dimensionality reduction method and a support vector machine (SVM) algorithm to quickly classify the spectrum of special steel materials. This approach enabled special steel types to be identified with 100% accuracy at high speed. Liu et al. [9] combined LIBS with PCA and SVM algorithms to classify and identify 20 plastics, and Gazeli et al. [10] proposed the use of linear discriminant analysis with LIBS technology to achieve efficient and rapid classification of olive oil. Li et al. [11] proposed a multivariate statistical method combined with LIBS for the complete discrimination of soft tissues such as fat, skin, and muscle. As a representative deep learning algorithm, convolutional neural networks (CNNs) rely on a parameter-sharing mechanism for high efficiency and accuracy in feature selection and neural network training. This structure produces powerful advantages in the calculation of high-dimensional data.

This article proposes a discrimination model combining PCA with a CNN for the differentiation of bauxite samples. The CNN structure is used with LIBS technology to realize the identification and classification of ten kinds of bauxite. To evaluate the proposed model, separate classifiers based on k -nearest neighbors (KNNs), random forest (RF), SVM, and full-spectrum feature inputs are constructed, and the classification performances of the various models are compared.

Experimental methods. A schematic diagram of the LIBS apparatus is shown in Fig. 1. The laser source uses a Quantel Nd:YAG laser. The seven-channel Echelle mid-step intensified charge-coupled device (iCCD) high-resolution spectrometer has a resolution of less than 0.09 nm, and can cover a spectral range of 190–950 nm. The focal length of the focusing lens is 30 mm. The sample is placed on a three-dimensional, electronically controlled translation stage. The XYZ axes of the sample stage are controlled by a computer.

All bauxite samples used in this study were provided by Jinan Zhongbiao Technology Co., Ltd. There are ten different bauxite samples: sample 1 – GBW(E)070169; 2 – GBW(E)070170; 3 – GBW(E)070171; 4 – GBW(E)070172; 5 – GBW(E)070173; 6 – GBW(E)070174; 7 – GBW(E)070175; 8 – GBW(E)070176; 9 – GBW(E)070177; 10 – GBW(E)070178. We take 3 g of the dried sample and use a 20-MPa, 150-s tablet press to form round samples with a diameter of 2 cm.

An optimization experiment determined the optimal laser wavelength to be 1064 nm, with a laser energy of 70 mJ, a laser focus spot size of 70 μm , a repetition frequency of 2 Hz, and a delay time of 1 μs . Each bauxite sample was divided into 15 compressed subsamples, and 20 sets of spectral data were randomly obtained from each subsample. Nine of these data were averaged across all groups to provide the repeatability requirement. The ten aluminum alloy samples therefore produced a total of $10 \times 15 \times 20 = 3000$ sets of spectral information. Among them, 60% (1800) of the samples were placed in the training set, 30% (900) of the samples were placed in the prediction set, and the remaining 10% (300) of samples formed the test set.

$$\sigma = \sqrt{\sigma^2} = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2}, \quad (6)$$

where $\bar{x}$ is the mean of the sample and σ is the standard deviation among all samples.

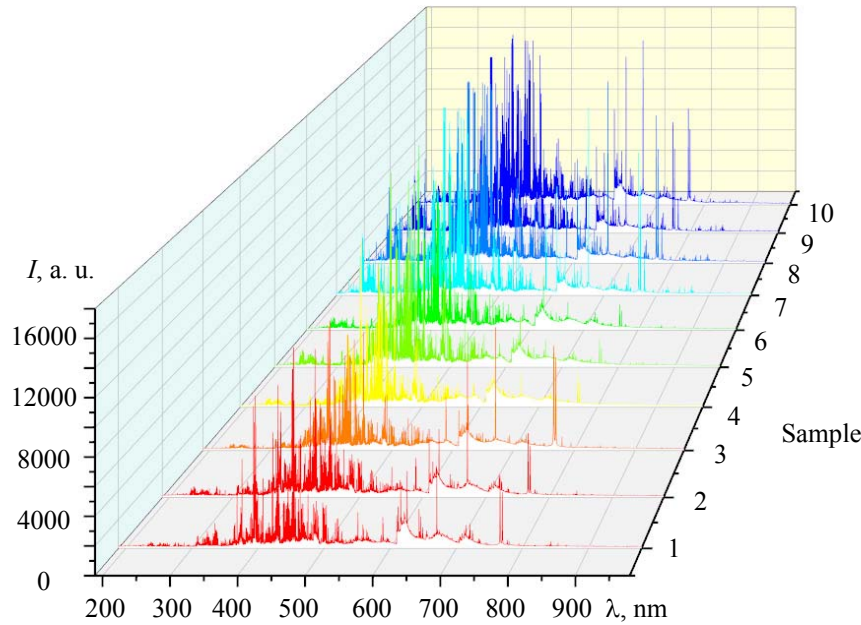


Fig. 2. LIBS spectral data and characteristic analysis of ten bauxite samples.

The spectrometer collected a total of 12,248 spectral points for each sample from 190 to 950 nm. Thus, there are 12,248 spectral feature variables in the model input tensor dimension, which makes model training very difficult. PCA can be used to reduce the dimensionality of the sample data. For the CNN structure, the input data form an 18×18 matrix. Therefore, after dimensionality reduction, the number of feature points is reduced from 12,248 to 324. With these 324 principal components, the cumulative contribution rate of variance reaches 99.6%, fully reflecting the information of the original bauxite samples. A ten-fold cross-validation method is used to verify the data to ensure the reliability and generalization ability of the experimental results.

Model construction and optimization. The CNN data are inputted in the form of a matrix. The construction method is shown in Fig. 3. The input tensor passes through the convolution, pooling, fully connected, and soft-max operations to produce the prediction results. The parameters are then iteratively optimized through stochastic gradient descent in the backpropagation step. In the process of building the network model, we determine the best classification effect by changing the parameters and structure of the CNN and analyzing the model performance on the verification set. We consider models with 2, 4, 8, 12, 16, and 20 convolution kernels. The CNN applies the convolution and pooling operations to the input matrix once. The average size of the convolution kernel is 3×3 and the pooling layer size is 2×2 . Features are extracted through maximum pooling with a learning rate of 0.01, batch size of 256, and rectified linear unit (ReLU) activation functions. After 100 training epochs, the accuracy and loss rate of the model tend to converge. When the number of convolution kernels is 20, the classification accuracy reaches 97.40%. The results in Fig. 4 show that a higher number of convolution kernels enables deeper extraction of data features and produces higher classification accuracy.

To further improve the classification accuracy, we design a CNN structure that performs convolution and pooling twice to deepen the feature extraction of the data. The numbers of convolution kernels in the first and second layers are 20 and 40, respectively. The classification accuracy of the test set reaches 99.6% using this structure. The results show that repeated convolution pooling can identify deeper features of the data, which is conducive to the accurate classification of samples.

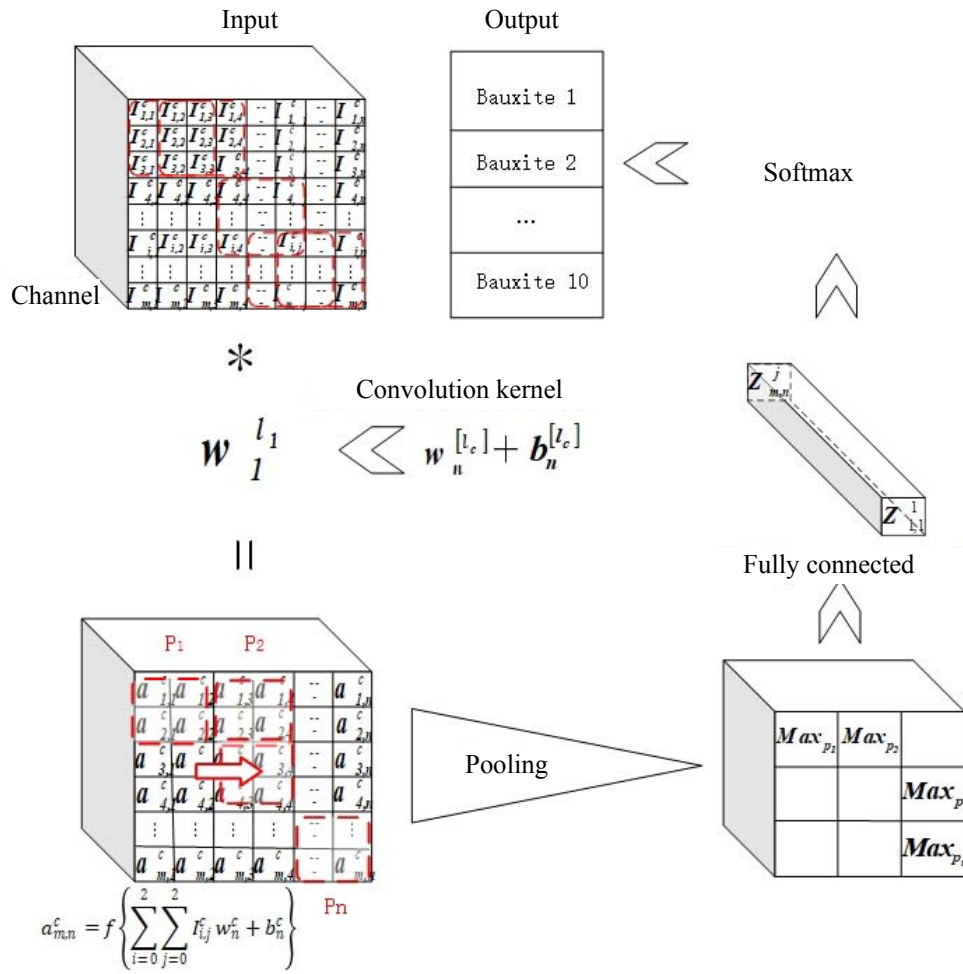


Fig. 3. Dimensional CNN model construction.

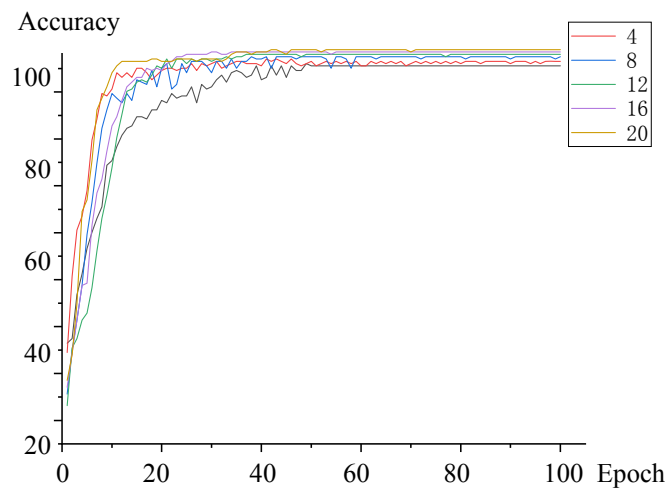


Fig. 4. Accuracy rate with different numbers of convolution kernels.

Comparison with other models. We also combined several common machine learning models with PCA to classify and identify the same bauxite samples. The classification results of KNN, RF, SVM, and full-spectrum feature input CNN models are compared with those of the proposed method in Table 1. The exper-

imental results illustrate the reliability and advantages of CNNs. Clearly, the proposed PCA-CNN model has the strong ability to recognize and generalize bauxite, and achieves excellent classification accuracy.

TABLE 1. Comparison of Different Models

Model	PCA-CNN	ALL-CNN	PCA-SVM	PCA-RF	PCA-KNN
Accuracy, %	99.60	96.58	95.18	94.80	93.70
Sensitivity, %	99.09	96.84	95.42	94.28	93.93
Precision, %	99.22	96.98	95.94	94.36	93.34

Conclusions. This paper has described a CNN combined with PCA-assisted LIBS for the accurate identification and classification of ten different bauxite samples. First, the Z-score method is used to standardize the original spectral data, and the standardized data are processed by PCA for feature reduction. The structure of the CNN is then designed, and the features of the input data are extracted multiple times through convolution and pooling operations. The experimental results show that the classification results are improved by subjecting the input variables to multiple convolution and pooling operations. The classification accuracy of the CNN reaches 99.6%. KNN, RF, SVM, and full-spectrum feature input CNN models were also used to classify and identify the same bauxite samples. The results show that the proposed PCA-CNN method outperforms these other models. In summary, CNN-assisted LIBS technology can accurately identify and classify different types of bauxite.

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