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Deep machine learning for STEM image analysis

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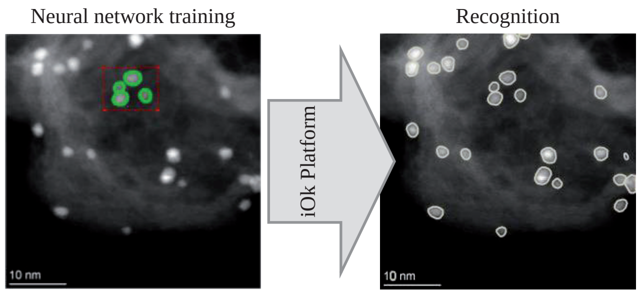
The universal, user-friendly online iOk Platform for automatic recognition of any type of objects in images based on deep machine learning is presented. Services aggregated in the iOk Platform significantly reduce the time spent on quantitative image analysis, decrease the influence of the subjective factor and increase the accuracy of the analysis by expanding the set of data that can be analyzed automatically. It is shown how the services can be used to analyze scanning transmission electron microscopy images obtained in heterogeneous catalysis studies, allowing for measurements of thousands of objects in an image, as well as simultaneous analysis of objects of different types, namely: nanoparticles and single sites.



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Deep machine learning for automatically finding, counting and measuring objects in any type of image, including images obtained using various types of microscopy, is already a powerful tool in modern research work.[1–10] Since the sizes of species responsible for catalytic activity (active component particles, single sites, *etc.*) are extremely important,[11,12] the application of this approach in heterogeneous catalysis is very useful.[11–14]

This article introduces the iOk Platform,[†] which provides access to the ParticlesNN website and the DLgram and No Code ML cloud services. Detailed instructions for using the ParticlesNN[9,10] and DLgram[15] services are available elsewhere. ParticlesNN and DLgram use the Cascade Mask-RCNN family[16] of neural networks pre-trained on the COCO dataset,[17] while No Code ML uses the ConvNeXt[18] neural network.[‡]

The image recognition results are provided in a graphic file with outlined contours and a JSON file in the LabelMe[19,20] program format. Outputting the result to a JSON file is an important feature of the developed services, as it gives the expert the right of the final decision when identifying objects: it is possible to correct the found contours, delete falsely found contours or add a missing one. The 'Calculate Stat' function of the modified LabelMe program[§] generates a table of object parameters required for statistical analysis. The user receives a list of object parameters (in pixels): area (S), diameter of the projected area [$D = 2\sqrt{(S/\pi)}$] and position (coordinates of the center) of each found object. This allows determining the mean size of an object and the distances between objects, calculating the number of objects per unit area of the image and building histograms of the size distribution. The development of the methodology for using previously developed services, as well as the experience of solving real practical cases, have shown that the ability to train neural networks by users on their own images makes the DLgram and No Code ML services universal and suitable for images of any type. The fundamental issue is the labeling of images for the training dataset. The advantages and disadvantages of the proposed approach lie in the basic principles of deep machine learning. In the extreme case of the most successful training, the network should see exactly what the user's eye sees, and should not see what the user does not see. The main disadvantage is the dependence of the recognition result on the quality of the training dataset. If the recognition result does not satisfy the user, then it is necessary to work with the correct labeling of images for training the network, as shown below.

The development of scanning transmission electron microscopy (STEM) poses new analysis challenges for researchers working in all fields of knowledge, including the investigation of supported catalysts. The huge number of visible particles in a single image is a difficult task for manual analysis. The use of neural networks has specifics regarding data labeling. Figure 1(*a*) shows the labeling of a STEM image of the Pd/Sibunite catalyst for training a neural network in DLgram. In a particular case, two crops were marked in regions with different contrast for better recognition. The training dataset consists of only 42 particles. Figure 1(*b*) shows the recognition result. It is clearly seen that all particles are well recognized: a total of 660 nanoparticles were found. The network falsely 'found' objects on the reference mark, but this is easily corrected in the LabelMe program. The analysis time is

[†] The iOk Platform is available at https://iok.nsu.ru/english/.

[‡] All of these services provide access to neural networks running on an HPE Apollo 6500 Gen10 server with eight NVIDIA Tesla V-100 graphics accelerators at the Institute of Intellectual Robotechnics at Novosibirsk State University.

[§] The modified LabelMe program is available at https://t.me/nanoparticles_nsk/10115.

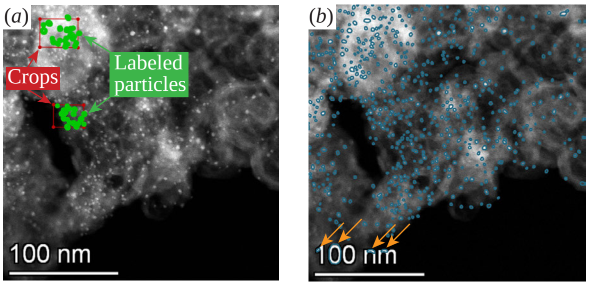

Figure 1 Object recognition using DLgram: (*a*) overview STEM image of Pd/Sibunite catalyst labeled for neural network training with red rectangles for crops and green contours for nanoparticles; (*b*) recognition result in the form of blue contours for recognized nanoparticles (brown arrows indicate incorrectly recognized objects).

reduced to minutes, and the model formed during the network training can be used to recognize similar images.

Recently, special attention has been paid to the consideration of single atoms and small clusters of the active component of catalysts (the so-called 'single sites') in the study of the mechanisms of catalytic reactions.[13,14] For this purpose, the problem of simultaneous analysis of nanoparticles and single sites should be solved. This can be done by labeling two types of objects for training the neural network. In the case shown in Figure 2, three crops were marked. The dataset consists of one nanoparticle and 31 single sites. Seven particles and 283 single sites were recognized [Figure 2(*b*)]. One particle was classified as both a 'particle' and a 'single site', which is easily corrected in the LabelMe program. Obviously, not all small objects can be recognized by the neural network in such images of real catalysts, since not all of them can be clearly detected by the researcher's eye. Since the sizes of such single sites are close to the resolution limit of the microscope, this problem can only be solved by further improving the setups and experimental conditions.

In conclusion, it should be noted that the described approach allows to significantly increase the volume of processed data in a fully automatic mode, saving researchers' time and significantly expanding the list of tasks to be solved. Modern progress in microscopic technology requires the use of deep neural networks for data analysis. The iOk Platform is a free and user-friendly image recognition tool that does not require coding skills and is available to researchers around the world.

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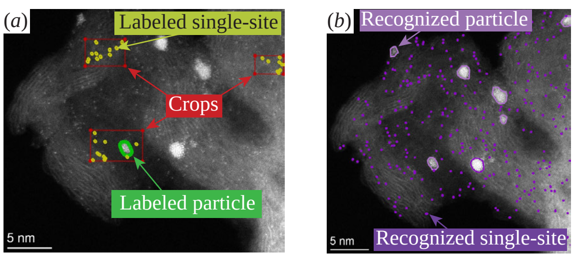

Figure 2 Object recognition using DLgram: (*a*) STEM image of Pd/Sibunite catalyst labeled for neural network training with red rectangles for crops, green contours for nanoparticles and yellow contours for single sites; (*b*) recognition result in the form of light lilac contours for nanoparticles and purple contours for single sites.

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