JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 16 No 6, 06008(6pp) (2024)
ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 16 № 6, 06008(6cc) (2024)

REGULAR ARTICLE

Novel Framework for Enhanced Nanoparticle Detection in Scanning Electron Microscopy Using Synthetic Data

G. Kumar[1,*], S. Kumar[2], A. Sharma[3], A. Raturi[4], A. Shrivastava[5], A.L.N. Rao[6], A.K. Khan[7]

[1] *Chitkara Centre for Research and Development, Chitkara University, Himachal Pradesh,174103, India*
[2] *Centre of Research Impact and Outcome, Chitkara University, Rajpura-140401, Punjab, India*
[3] *Department of Mechanical Engineering, GLA University, Mathura- 281406, Uttar Pradesh, India*
[4] *Department of Mechanical Engineering, Graphic Era Deemed to be University, Dehradun, India*
[5] *Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, Chennai, TN, India*
[6] *Lloyd Institute of Engineering & Technology, Greater Noida, India*
[7] *Lloyd Law College, Greater Noida, India*

(Received 27 August 2024; revised manuscript received 20 December 2024; published online 23 December 2024)

Nanoparticle detection in scanning electron microscopy (SEM) is crucial for various applications. Existing techniques for detecting nanoparticles in SEM images need help to handle dispersed particles and need more accuracy. This research uses a deep learning strategy to enhance recognition efficiency and precision. To overcome the challenges, we develop a robust Multi fused Spectral Deep Convolute Neural Net (MS-DCNN) based model for nanoparticle detection, utilizing synthetic data generation to facilitate practical neural network training and collecting the SEM image dataset for detecting the nanoparticle. Created an algorithm to generate synthetic data, combining random particle distributions to simulate SEM micrographs and allows the development of annotated datasets that are essential for neural network training. Compared to existing approaches; the results are reduced pixel (0.62), warp errors (0.0008), decreased computing time (398s) and greater accuracy (92.5%). The suggested MS-DCNN framework is practical and better than conventional techniques, exhibiting improved precision in the identification of dispersed nanoparticles. The generation of synthetic data helps in the development of a trained model that will deal with a variety of particle distributions. The model is trained using synthetic data, demonstrating the technique's potential to improve nanoparticle analysis in SEM imaging which got proven result over the existing method.

Keywords: Nanoparticle, Scanning Electron Microscopy (SEM), Synthetic Data, Multi fused Spectral Deep Convolute Neural Net (MS-DCNN).

DOI: 10.21272/jnep.16(6).06008 PACS numbers: 61.46.Df, 68.37.Hk

1. INTRODUCTION

Detection of nanoparticles by scanning electron microscopy (SEM) was essential to many scientific fields, such as biology, materials science and nanotechnology [1]. The characteristics of nanoparticles and maximizing their uses require accurately identifying and describing them. Due to the small size and tendency for aggregation, nanoparticles present intrinsic obstacles in their detection, making new techniques that are necessary to improve detection sensitivity and accuracy [2].

1.1 The Importance of Detecting Nanoparticles

The structure, distribution and behaviour of nanoparticles require accurate detection of these particles. Understanding environmental interactions, evaluating the effectiveness of medicine delivery systems and enhancing material qualities benefit from the knowledge [3]. Improving the detection of nanoparticles not only accelerates research but also helps create cutting-edge technology with a wide range of applications.

1.2 Difficulties in Detecting Nanoparticles

Noise changes in nanoparticle morphology and a lack of available datasets for algorithm training are problems with traditional SEM-based nanoparticle detection techniques. When working with multifaceted nanoparticle samples, overcoming these obstacles was essential to achieve reliable and effective detection [4].

1.3 Solution of Synthetic Data

* Correspondence e-mail: gauravcivilengg714@gmail.com

Cite this article as: G. Kumar et al., *J. Nano- Electron. Phys.* 16 No 6, 06008 (2024) https://doi.org/10.21272/jnep.16(6).06008

The intriguing way to overcome the drawbacks of conventional detection techniques was to employ synthetic data. To train detection techniques on a controlled and varied sample set, synthetic datasets that imitate real-world SEM images can be created [5]. Improved performance across a range of sample types and experimental settings can be achieved by utilizing synthetic data to strengthen the generalizability and resilience of nano-particle detection models. The scope of the research used MS-DCNN detection strategy for the purpose of identifying dispersed nanoparticles in SEM images. Computer software was created to create digital pictures that resembled SEM micrographs, representing the nanoparticles present in the actual sample, to acquire annotated training data.

The structure of the article is as follows: The article is divided into five parts: Part 2 covers relevant work, Part 3 describes the materials and techniques used in the suggested algorithms, Part 4 shows the results of the performance evaluation and Part 5 concludes.

2. RELATED WORKS

In the study, a unique Deep Learning technique for automated nanoparticle detection, classification, orientations inference and reconstruction in three dimensions from microscope images was presented. The method makes use of convolutional neural networks (CNN) [6]. The approach has limits in terms of portraying real-world variability and processing demands as well as exhibits promising results when used with generated datasets that mimic images from a scanning electron microscope. It provided an effective method for nano-particle characterization. To overcome the lack of algorithms in nanotechnology, the study developed an extensive framework for nanoparticle categorization in SEM images. The model attained an impressive 97% accuracy and 98 % F1-score by combining morphological procedures [7], Visual Geometry Group 19 (VGG-19) deep networks and Gray Wolf Optimization (GWO). There were imbalances in the dataset, but the study highlights the promise of the model as an effective tool for nanoparticle analysis. There were issues with generalizability and processing needs. To categorize and segment nanostructured materials in TEM images, the study [8] used Mask R-CNN (Region-SNN) with Residual Network 101(ResNet) 101. For hydrogen silicate, silicon dioxide nano-particles and coating compounds, the research achieved remarkable accuracy scores of 85-99%. Although issues with generalizability and real-world artifacts remain, the model performs well in identifying overlapping clusters, demonstrating its potential as a reliable tool for nanomaterial investigation.

The Cascades Mask-RCNN neural network was used in the study [9] to automate the recognition of nanoparticles in TEM images of heterogeneous catalysts. With low deviation from manual assessment, the integrated 'Particles NN' online service accelerated TEM data processing, decreasing analysis time to minutes and achieved recall and precision of 0.71 for both types of objects and 0.84 for visible particles. The instrument improved the accuracy and objectivity of catalytic research. To examine the atomic framework of PtNiPdCoFe images of alloys with high entropy (HEAs) obtained with a scanning electrons transmission microscopy (STEM), the study [10] proposed a fully convolutional neural network (FCN). In elemental atomic fractions, the DL model provides precise column height estimates that highlight local aggregations and non-uniform fluctuations. Potential sensitivity to laboratory conditions and the requirement for additional generalization testing were among the limitations.

With an emphasis on electron microscopy, the article [11] investigated an upsurge in the use of deep learning-based object recognition models in materials science. A community-curated ecosystem was envisioned to improve object detection's broader application in other materials areas. A CNN was developed in the study to detect measurements of the height of atomic column in excellent quality TEM images containing particles of gold in real-time [12]. With the use of a regression technique and a physically real-world training dataset produced by the William Wulff development, the CNN rapidly and precisely extracts conditions from experiments. While generalizability and practical variability were the important factors to consider, the paradigm lays the groundwork for expedited nanoparticle analysis in nanoscience.

To provide accurate nanoparticle modelling, the paper [13] integrated a novel protecting model into an expedited approach for characterizing the structure of nanoparticles using generated datasets. A generative adversarial network for improving resolution in SEM images was presented in the article [14-15]. The method offered significant efficiency enhancements in SEM imaging by allowing for faster acquisition of images with more excellent resolution while mitigating the electron imposing and sample damage.

3. PROPOSED METHODOLOGY

Creating a MS-DCNN, especially for SEM images, is the suggested technique. To imitate SEM micrographs, synthetic data collection is applied, which makes it easier to provide a variety of structured data sets for efficient MS-DCNN training. Multi fused convolutional layers are used in MS-DCNN design for feature extraction, whereas fully linked layers are used for classification. The algorithm uses these artificial datasets to improve the model's nanoparticle detection performance. Evaluation measures are used to compare the model's performance with other approaches, such as accuracy, computation time, pixel error and warp error.

3.1 Data Collection

The dataset includes descriptions of the relevant three-dimensional (3D) structures for 2048 synthetic SEM images of powder materials. Each set consists of 256 systems and images that are grouped according to eight closely similar particle size distributions (PSDs).

3.2 Synthetic SEM Images

Blender is an open-source graphics program used for scientific visualization, rendering, animation and 3D modelling. It was used to create the dataset. The spherical particles that comprise the powder structures are selected at random from the designated PSDs. A total of 2048 synthetic powder microscopy images were produced by creating 256 individual structure/image pairings for each of the eight unique PSDs. Each image was created by placing 800 particles into an $11 \times 11 \times 2$ (arbitrarily Bender units) render container. Using one of the eight producing PSDs, randomly chosen particle radii were used to provide for particle occlusions and intersections. A spherical model was used to generate the particles and an image of zinc grains from the dataset was used to give them a surface texture. Fig. 1 shows the two-step procedure for creating particle images. There are two processes in the creation of a synthetic image. JSON files with information on every particle in the image are made in the first phase (a). Then, textured images are produced in step (b) of the process, where textures are selected from a database of actual SEM images. After the generation stage, each image is subjected to a 5×5 pixel histogram normalizing process, which is carried out to improve the general quality and visual coherence of the images of manufactured nanoparticles.

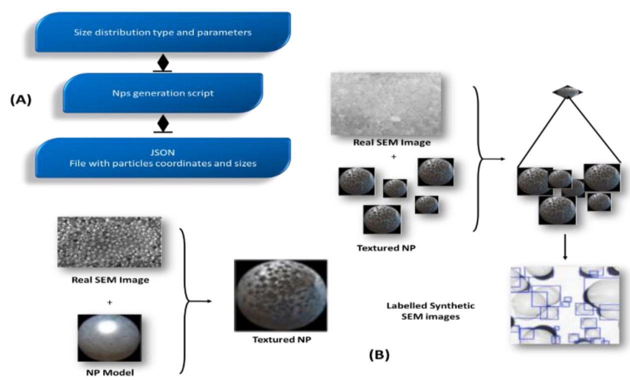

Fig. 1 – Procedure for creating particle images

3.3 Data Preprocessing

Histogram equalization data preparation is a method used to improve contrast and feature visibility in images, when using synthetic data for nanoparticle identification in SEM. By modifying the proportions of pixel intensities in an image, the technique improves its suitability to use with later image analysis techniques. Histogram equalization is applied to enhance the detection of nanoparticles, which entails a mathematical adjustment of the image's values of intensity to produce a more uniform histogram. The density function of probability *$k(V_r)$* for the image Vis expressed in Eq. (1).

$$k(V_t) = \frac{n^t}{n} \tag{1}$$

For each value of t in the range of $t = 0, 1, \ldots, L-1$. Where n is the periodicity at which the intensity level (V_t) occurs and n^t is the total number of pixels in the input picture V. The input picture's histogram is associated with $k(V_t)$, which denotes the number of pixels with a particular intensity V_t. In actuality, n^t versus V_t is represented graphically by the V histogram. Eq. (2) illustrates how the density function of probabilities is used to express the cumulative density function.

$$C(V) = \sum_{x=0}^{t} k(V_x) \tag{2}$$

The $C(V_{(L-1)})$ must inevitably equal 1 when V_t is equal to w for any t range from 0 to $L-1$. To transfer the input image into the whole dynamic range denoted by (V_0, $V_{(L-1)}$), the method (HE) employs the average density function as the transformation function. Let's construct the transformation functional $f(v)$ as given in Eq. (3), building on the accumulating density function.

$$f(v) = V_0 + (V_{L-1} - V_0)C(v) \tag{3}$$

Eq. 4 and 5 enable us to express the HE's output image as $y = y(i, x)$.

$$y = f(V) \tag{4}$$

$$= \{f(V(i,x)|\forall\, V(i,x)\epsilon V\} \tag{5}$$

HE stretches the intensity values throughout the whole range, making details in an image more accessible to identify in low-contrast areas. It's a robust approach. Use caution when applying it, as its efficacy varies depending on the image's properties and the particular objectives of the image processing assignment.

3.4 Multi fused Spectral Deep Convolute Neural Net (MS-DCNN)

A MS-DCNN is a crucial component in the field of better nanoparticle identification in SEM utilizing synthetic data. The neural network is designed to interpret complex characteristics and patterns found in SEM images of nanoparticles. It operates as a sophisticated image-processing architecture. Convolutional and pooling layers are two of the many layers that are included in its architecture to extract complicated characteristics from raw pixel input hierarchically. The network uses training data to forward propagation, which produces a loss function that measures the difference between expected and actual values. To maximize the neural network's performance, backpropagation modifies its parameters according to the derivatives of the loss. The complete architecture, which combines FPN in Retina Net with a pre-trained backbone, demonstrates a reliable method of object recognition that places a focus on the extraction of features and precise predictions. The neural network passes through an essential step in the training phase when the loss function, which shows the difference between expected and actual results, is calculated. During backpropagation, the network parameters are adjusted in a manner that is proportional to the variations of the loss concerning these parameters. For Retina Net, in particular, using Focal Loss is a valuable training technique. Before each cycle, the augmented pictures are randomly sheared, rotated and flipped along with their respective bounding boxes to train the neural network. This training program runs for around 50 hours on the Kaggle cloud GPU (NVidia K80), covering 48 epochs with an initial batch size of 16. The optimizer developed by Adam is used and the acquisition rate is fixed at 0.001. Fig. 2 shows the schematic of the training process, which gives a visual picture of the complexities involved.

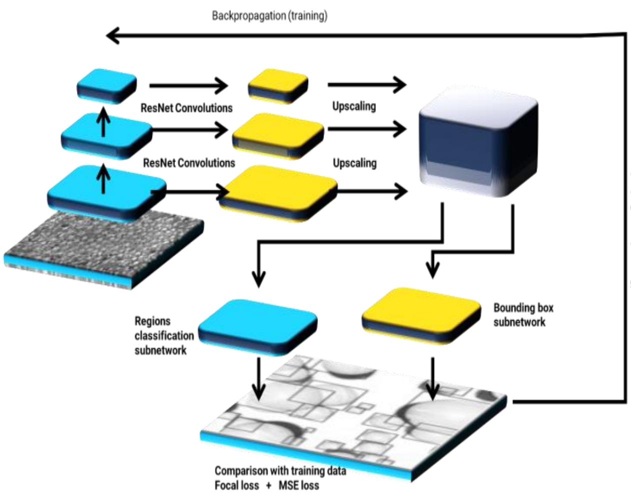

Fig. 2 – Structure detection of nano participles

4. RESULT AND DISCUSSION

The hardware specs used during the training stage were the same ones used for the test evaluation. The machine was equipped with an Intel Core i9 processor running at 3.60 GHz and an NVIDIA GeForce RTX 2080 GPU with 8 GB of RAM. Furthermore, the device included 32 GB of RAM. By minimizing possible differences brought by hardware discrepancies, this uniformity in hardware configuration throughout the training and testing stages helps to assure an accurate and fair evaluation of the model's performance.

The efficiency of the suggested strategy is evaluated by using a number of common existing approaches such as Inception – V3, ResNet, Inception – V4, UNet and GAN [19, 20]. A number of metrics are used to evaluate the system's performance, including pixel and warp errors, accuracy and calculation time, all of which are covered in more detail in the sections that follow.

Accuracy

Accuracy is a performance parameter used in SEM to assess the overall accuracy of the detection strategy in the context of nanoparticle detection. The ratio of properly recognized nanoparticles (true positives) to all nanoparticles, both effectively and erratically identified, is used to measure accuracy. The following is the accuracy Eq. (6).

$$Accuracy = \frac{Number\ of\ True\ Positives}{Total\ Number\ of\ Nanoparticles} \tag{6}$$

Table 1 – Values of Accuracy

Methods	Accuracy (%)
Inception – V3	89.8
ResNet	87.5
Inception – V4	89.2
Proposed	92.5

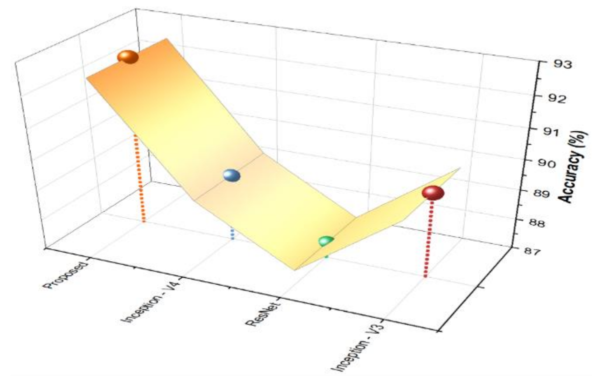

Fig. 3 – Comparison of Accuracy

Fig. 3 and Table 1 depict the comparison of accuracy. The suggested technique (92.5 %) outperforms the current oneslike Inception – V3 89.8 %, ResNet 87.5 % and Inception – V4 89.2 % [19], exhibiting increased precision in the identification of nanoparticles in SEM images. This improved performance highlights the method's usefulness and demonstrates its effectiveness as a valuable instrument for improved and accurate nanoparticle identification in SEM applications.

Computation Time

Computation time in SEM nanoparticle detection is the amount of time the detection model needs to process and analyze images from SEM to detect and recognize nanoparticles. It is an important statistic that indicates how effective the detection technique is for real-time and practical applications; shorter calculation durations are preferred. In the detection of nanoparticles (Eq. 7), the computation time (T) can be represented as the difference across the time at the start of the process (t_{start}) and the time at the conclusion (t_{end}) of the method of detection (t_{end}).

$$T = t_{end} - t_{start} \tag{7}$$

Table 2 – Values of computation time

Methods	Computing Time(s)
Inception – V3	434
ResNet	7018
Inception – V4	6135
Proposed	398

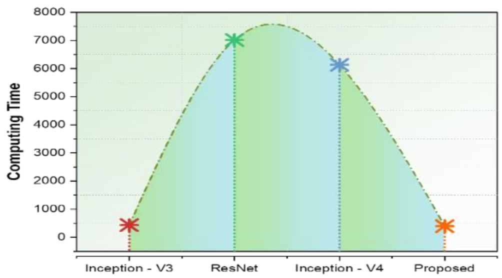

Fig. 4 – Outcome of computation time

Table 2 and Fig. 4 depict the outcome of computation time. The suggested approach is positioned as a very beneficial tool due to this efficiency improvement, which makes it useful for the rapid and precise detection of nanoparticles in SEM techniques.

5. CONCLUSION

They study to improve effectiveness and accuracy by using a deep learning technique to overcome the difficulties associated with nanoparticle identification in SEM. The neural network had been trained by creating synthetic data and developing a robust MS-DCNN-based model. Identified datasets are vital for training and the system created SEM micrographs with a variety of particle distributions. An investigation of comparisons revealed that the suggested MS-DCNN framework outperformed current methods in terms of pixel (0.62) and warp errors (0.0008), computation time (398s), as well as accuracy (92.5%). Though there could be some drawbacks, such as difficulties in reproducing intricate particle configurations, the study provides encouraging perspectives. To further improve nanoparticle identification abilities using SEM imaging, the future scope entails improving the synthetic data creation process, investigating more extensive coupled with diversified datasets and incorporating developments in deep learning approaches.

REFERENCES

1. J. Rydz, A. Šišková, A. Andicsová Eckstein, *Adv. Mater. Sci. Eng.* **2019**, 6871785 (2019).
2. M. Zhang, J. Yang, Z. Cai, Y. Feng, Y. Wang, D. Zhang, X. Pan, *Environ. Sci.: Nano* **6** No 3, 709 (2019).
3. L.K. Hakim, M. Yazdanian, M. Alam, K. Abbasi, H. Tebyaniyan, E. Tahmasebi, D. Khayatan, A. Seifalian, R. Ranjbar, A. Yazdanian, *Evidence-based Complem. Alternative Med.* **2021**, 9011226 (2021).
4. A. Subramanian, K. Cruse, A. Trewartha, X. Wang, A.P. Alivisatos, G. Ceder, arXiv preprint arXiv:2112.01689 (2021).
5. O.M. Manyar, J. Cheng, R. Levine, V. Krishnan, J. Barbič, S.K. Gupta, *J. Comput. Inform. Sci. Eng.* **23** No 3, 030903 (2023).
6. A. Cid-Mejías, R. Alonso-Calvo, H. Gavilán, J. Crespo, V. Maojo, *Comput. Meth. Prog. Biomed.* **202**, 105958 (2021).
7. G. Dahy, M.M. Soliman, H. Alshater, A. Slowik, and A.E. Hassanien, *Comput. Mater. Sci.* **223**, 112135 (2023).
8. C. Cabrera, D. Cervantes, F. Munoz, G. Hirata, P. Juárez, D.L. Flores, *Neural Comput. Appl.* **34** No 13, 11035 (2022).
9. A.V. Nartova, M.Y. Mashukov, R.R. Astakhov, V.Y. Kudinov, A.V. Matveev, A.G. Okunev, *Catalysts* **12** No 2, 135 (2022).
10. M. Ragone, M.T. Saray, L. Long, R. Shahbazian-Yassar, F. Mashayek, V. Yurkiv, *Comput. Mater. Sci.* **201**, 110905 (2022).
11. R. Jacobs, *Comput. Mater. Sci.* **211**, 111527 (2022).
12. M. Ragone, V. Yurkiv, B. Song, A. Ramsubramanian, R. Shahbazian-Yassar, F. Mashayek, *Comput. Mater. Sci.* **180**, 109722 (2020).
13. L. Lin, Z. Wang, G. Yang, *Accelerating Nanoparticle Characterization Using Synthetic Sem Datasets and Deep Learning Techniques*. Available at SSRN 4524822.
14. K. de Haan, Z.S. Ballard, Y. Rivenson, Y. Wu, A. Ozcan, *Sci. Rep.* **9** No 1, 12050 (2019).
15. N. Ortiz Peña, D. Ihiawakrim, M. Han, B. Lassalle-Kaiser, S. Carenco, C. Sanchez, C. Laberty-Robert, D. Portehault, O. Ersen, *ACS Nano* **13** No 10, 11372 (2019).

Нова структура для покращеного виявлення наночастинок у скануючій електронній мікроскопії з використанням синтетичних даних

G. Kumar[1], S. Kumar[2], A. Sharma[3], A. Raturi[4], A. Shrivastava[5], A.L.N. Rao[6], A.K. Khan[7]

[1] *Chitkara Centre for Research and Development, Chitkara University, Himachal Pradesh,174103, India*
[2] *Centre of Research Impact and Outcome, Chitkara University, Rajpura-140401, Punjab, India*
[3] *Department of Mechanical Engineering, GLA University, Mathura- 281406, Uttar Pradesh, India*
[4] *Department of Mechanical Engineering, Graphic Era Deemed to be University, Dehradun, India*
[5] *Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, Chennai, TN, India*
[6] *Lloyd Institute of Engineering & Technology, Greater Noida, India*
[7] *Lloyd Law College, Greater Noida, India*

Виявлення наночастинок у скануючій електронній мікроскопії (SEM) має вирішальне значення для різних застосувань. Існуючі методи виявлення наночастинок на SEM-зображеннях потребують допомоги для обробки диспергованих частинок і потребують більшої точності. Це дослідження використовує стратегію глибокого навчання для підвищення ефективності та точності розпізнавання. Щоб подолати труднощі, ми розробили надійну модель детектування наночастинок на базі Multi fused Spectral Deep Convolute Neural Net (MS-DCNN), використовуючи генерацію синтетичних даних для полегшення практичного навчання нейронної мережі та збору набору даних зображень SEM для виявлення наночастинок. Створено алгоритм для генерації синтетичних даних, поєднуючи випадкові розподіли частинок для моделювання SEM-мікрофотографій і дозволяючи розробляти анотовані набори даних, необхідні для навчання нейронної мережі. Порівняно з існуючими підходами; результатом є зменшення пікселів (0,62), помилок деформації (0,0008), зменшення часу обчислення (398 с) і більша точність (92,5%). Запропонована структура MS-DCNN є практичною та кращою, ніж звичайні методи, демонструючи підвищену точність ідентифікації диспергованих наночастинок. Генерація синтетичних даних допомагає в розробці навченої моделі, яка матиме справу з різними розподілами частинок. Модель тренується з використанням синтетичних даних, що демонструє потенціал техніки для покращення аналізу наночастинок у SEM-зображенні, який отримав перевірений результат порівняно з існуючим методом.

Ключові слова: Наночастинки, Скануюча електронна мікроскопія (SEM), Синтетичні дані, Мультиконцентрована спектральна глибока згорнута нейронна мережа (MS-DCNN).