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Automated Analysis of Grain Growth Under in-situ Irradiation Using Convolutional Neural Network

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In-situ transmission electron microscopy (TEM) provides a unique opportunity to directly observe kinetic processes in materials. Meanwhile, a large number of images could be acquired during in-situ TEM experiments, making the data analysis process tedious and potentially biased. Therefore, it is highly desirable to establish capabilities for automated image analysis to improve the efficiency and consistency. In recent years, an exciting and powerful tool for analyzing microstructures in TEM images that have emerged and developed quickly is Convolutional Neural Network (CNN) because of its high accuracy for image classification and recognition. Nowadays, more and more studies have applied CNN to analyze microstructure evolution of materials under extreme environments [1][2]. In this project, we developed a CNN-based model for automated grain morphology analysis in TEM images of UO_2. In-situ Kr ion irradiation was conducted to investigate the radiation-induced grain growth of UO_2. During the experiment, thin films of UO_2 with nanograins were irradiated by 1 MeV Kr ions using the Intermediate Voltage Electron Microscopy (IVEM) facility at Argonne National Laboratory. Both dark-field (DF) and bright-field (BF) TEM images were acquired during the experiments and more than 100 TEM images were collected in total.

To process this large dataset, we first developed a model that can automatically recognize grains and measure the grain sizes in DF-TEM images. Our model is based on U-Net, which is a CNN model with a unique U-shaped architecture that makes it efficient in segmentation and particle analysis. There is a contracting path to extract image context and a symmetric expansive path to propagate context information to higher resolution layers [3]. Our model contains one input layer, one output layer, four max-pooling layers, four concatenate layers, and 23 convolutional layers. A schematic plot showing the model architecture is presented in Figure 1. a. A single NVIDIA Tesla P100 GPU was used to train the model to about 200 epochs with L2 Regularization. The training was terminated when the validation loss stops decreasing and only the best model during the entire training process was automatically saved. The total training time was about six hours. Since the size of training data plays a critical role in improving the U-net model performance, we used data augmentation to enlarge the dataset. As CNN relies on spatial information to tune the model parameters, methods like cropping, rotation, flipping, and scaling are simple but useful augmentation methods. Our original dataset contains 20 TEM DF images of 1024×1024 pixels and after data augmentation, the final dataset has 200 DF-TEM images in total. Compared to the models trained by the original dataset, the performance of the models trained by the augmented dataset increased about 4% in F1 score. Our DF U-Net model has successfully reached similar performance as human experts (see Figure 1. b). The developed model reached 97.46% in accuracy and 81.15% in F1 score for analyzing grains in DF-TEM images. Tests show that the developed U-Net model is about 2000 times faster than human experts in labeling images and it has been applied to accelerate the data analysis for understanding the radiation-induced grain growth in UO_2. The major limitation of the DF model is that overlapped grains cannot be separated.

The developed neural network model also showed the potential for processing BF-TEM images. Therefore, we collected a new dataset containing 350 augmented BF-TEM images of 1024×1024 pixels for training. However, the developed BF model did not achieve the same performance as the DF model. Overall the BF model has about 90% in accuracy and 70% in F1 score. Fig. 1c shows the processed result of a regular BF image with only a fraction of grain boundaries recognized. We noticed that the present BF model can reach a much better performance for BF-images with continuous and clear grain boundaries as shown in Figure 1. d, suggesting that the BF model could be further improved if a larger training dataset with higher quality is used. The training images used now were labeled by three researchers and their standards for labeling were not quite consistent, which may confuse the model. The quality of training images is being improved now and a new U-Net model is being developed for processing BF images and in-situ TEM videos.

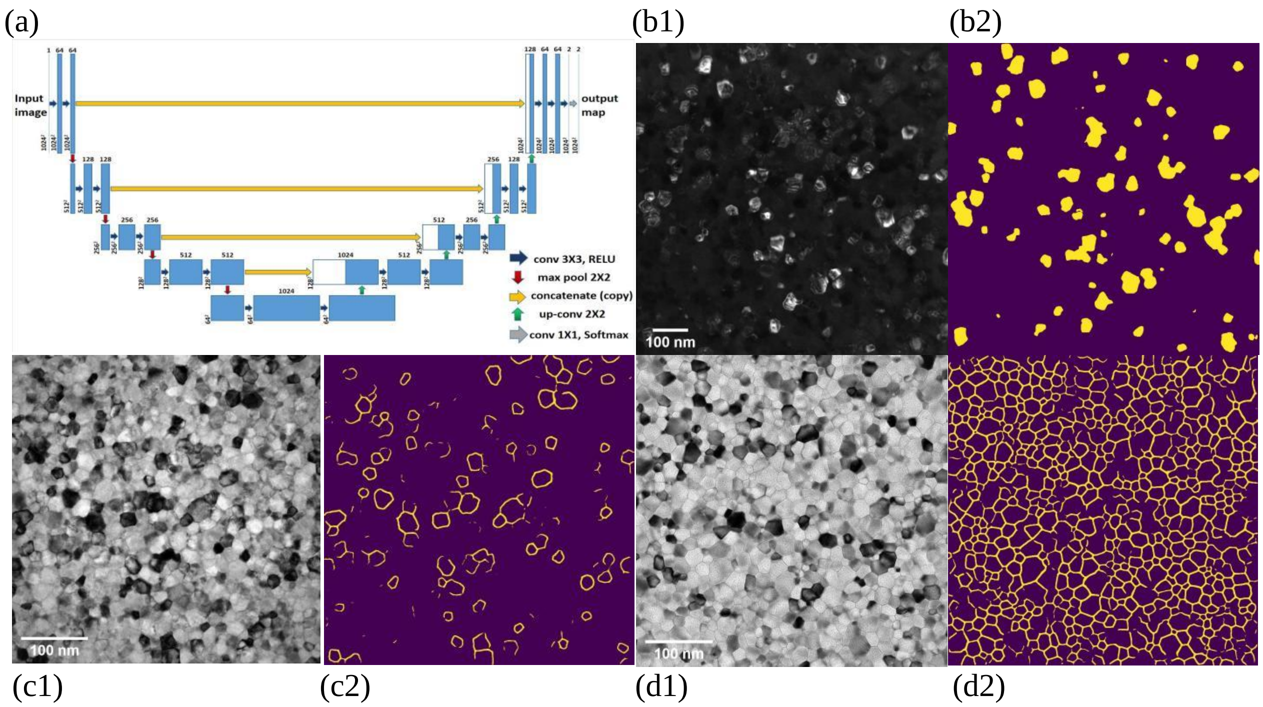

Figure 1. (a) U-Net Architecture used in this study; (b,c,d) Original TEM images and the corresponding labeled images by U-Net. TEM images are in gray scale. In the labelled results, grain or grain boundaries are highlighted in yellow.

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