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AFM Imaging Defect Detection and Classification with Artificial Intelligence and Deep Learning

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***Abstract*—Atomic force microscopy (AFM) is a powerful tool for investigating the topographical and mechanical properties of a wide range of samples. However, the process of data acquisition and analysis using AFM is time-consuming and labor-intensive, and can be prone to error. Mistaken imaging of the wrong sample, damage to the sample, and tip wear are just a few examples of potential sources of error. Currently, the integration of artificial intelligence (AI) with AFM operations for identifying and classifying sample images is still under investigation. In this paper, we propose a novel deep learning (DL) framework for the classification of AFM images. The key component of the proposed AI framework is a DL neural network model that is trained using the AFM images with various types of blemishes labeled by experts. Then the trained network will be used to analyze future AFM images of the same type of samples. Specifically, the proposed DL model consists of a defect detection layer and a feature extraction and classification layer to ensure the classification accuracy. The Performance of the proposed AI framework was demonstrated in terms of defect detection and classification accuracies in both training and validation. The proposed AI approach will greatly reduce the time and labor cost in AFM quality analysis, and can be potentially extended to other applications, such as manufacturing, material engineering, and biomedical engineering.**

***Index Terms*—AFM, deep learning, image analysis, identification, classification**

I. Introduction

As an important member of the "scanning probe microscope" family, the atomic force microscopy (AFM) [1] [2] is broadly used to investigate the surface structure and mechanical properties of solid materials. AFM is able to function in various environments, including low temperatures, liquids, a vacuum, and the atmosphere. AFM can capture the topography images of sample surfaces in three dimensions with high resolution. Although the superiority of AFM in terms force and time resolutions and versatility makes it a powerful tool [3] for material studies, this technique is time consuming and requires specific skill sets and constant human supervision. This is because AFM operations are often accompanied with such as cantilever tip breakage after prolonged functionalization and damage to the soft samples (like living cells) due to lack of optimization of the loading forces, which make this method low throughput. For example, the system cannot stop and report an error automatically. Instead, the experimentalist must manually screen and identify the defects for each sample image. Therefore, it is necessary to explore alternative methodologies in AFM applications to address these issues.

Remarkable progress in the area of artificial intelligence (AI) and deep learning (DL) over the past few years has left its mark on material imaging, especially in post processing and image analysis of various samples to enhance the quality of the data and process of material mechanical characterization. Over the past couple of years, researchers in the material science community have begun to combine AI approaches with AFM for various pattern recognition and data post processing tasks [4] [5] [6]. Furthermore, some initial research happened to select appropriate AFM scanning areas and data modeling using deep learning [7] [8]. However, these approaches are either limited to certain types of samples, or only focus on post operation data processing. Therefore, the integration of AI with AFM real-time operations are still under development. In this paper, an AI-enabled AFM operational framework is proposed to address the current AFM limitations in the image classification and identification of various samples, thereby reducing the labor and time cost.

In the proposed framework, AFM images are analyzed using DL-based object detection and localization methods to automatically select defect locations based on the user-selected defect shape. This idea will help the researchers significantly by speeding up the AFM experiments. Specifically, the proposed DL model consists of a defect detection layer, a feature extraction and classification layer. The DL model has been trained by a large data set of AFM images with various types of blemish shapes annotated by experts. Once trained, the DL network will be applied to detect and classify the AFM images in real time operations. In this work, the trained DL focuses on identifying and marking three distinct blemish shapes: scratches, wobbles, and cracks. As an example, the DL network model in this work chooses You Only Look Once (YOLOv5) [9] as the defect detector, and ResNet-34 [10] as the enhanced feature extractor and classifier. The former is known for its faster processing time, better detection accuracy, and more compact model size. The latter is specifically designed for feature extraction and identification classification. The output of the trained model includes both the type (e.g., shape) of the detected defect

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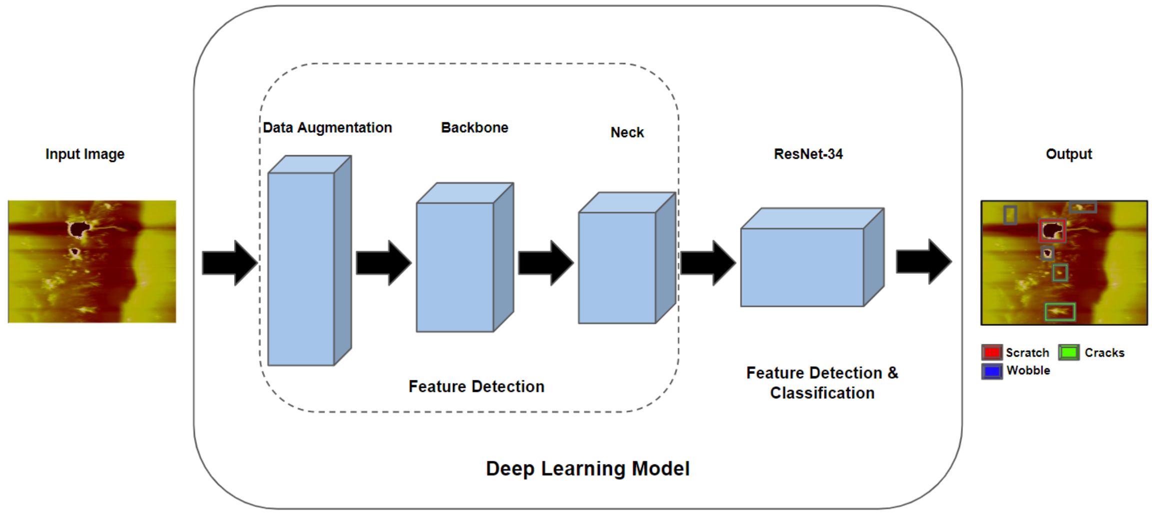

Fig. 1. Overview of the proposed AI AFM image classification framework.

and its location in the image, which can be further used for downstream sample analysis and decision-making. In addition, the proposed AI framework is made available for users to add newly classified AFM images to the DL model database to improve the model's accuracy and versatility. This feature enables the model to learn from new and diverse sample images, thus enhancing its capability to detect and classify various blemish shapes.

The proposed AI framework has been validated and tested using AFM images acquired from samples with complex features. The high validation accuracy demonstrates the potential of using DL-based approaches for defect detection and quality control in AFM applications. It also provides a comprehensive pipeline for implementing such approaches in practice.

II. Methods

An overview of the proposed AI framework is illustrated in Fig. 1.

A. AFM Image Data Collection

The collected AFM sample topography images serve as the foundation for training our DL model and validating the overall framework. All AFM images that were used for the training and validating the proposed DL model were acquired during the topography imaging of various samples by using commercial AFM systems (such as the BioResolve and Dimension Icon AFM systems by Bruker Nano. Inc.). An automatic script function in Python was written to convert the raw AFM .spm files to jpeg images for the purpose of reducing computation time of the DL model.

B. DL Model for Defect Detection

We utilized a state-of-the-art DL neural networkmodel to achieve capabilities beyond traditional DL object detection tasks, and trained it to detect various defect shapes in AFM topography images.

1) Architecture of the DL defect detection model: the DL model focuses on the detection of the presence of imaging defects (blemishes) and classification of the common defect types, such as cracks, scratches, and shakes, which are commonly encountered in AFM applications. As shown in Fig 1, the proposed DL model contains two key components: a defect detector and a feature extractor and classifier.

The defect shape detection and localization could be achieved using a framework with real-time object detection, such as the You Only Look Once (YOLO) algorithm [11]. YOLOv5, newest edition, is used in this work, which is a relative new version of the YOLO series and has several improvements over its predecessors, including faster processing times, better accuracy, and larger compact model size. It is primarily designed for object detection, which involves image feature detection and object localization. Specifically, YOLOv5 uses a single convolutional neural network [12] to perform both tasks by dividing the input image into a grid of defects and using each defect to predict the presence and location of objects in its area. Each grid cell predicts multiple bounding boxes along with their positions and dimensions, the probability of an object in the underlying grid, and conditional class probabilities. The class probabilities are used for defect classification, and the bounding boxes are used for defect localization. Thus, while YOLOv5 is primarily designed for object detection, it can also perform image classification to a certain extent by using the class probabilities output of the network. However, it is less suitable for image classification than other architectures, such as ResNet [13], specifically designed for image classification tasks.

The ResNet architecture is known for its ability to train

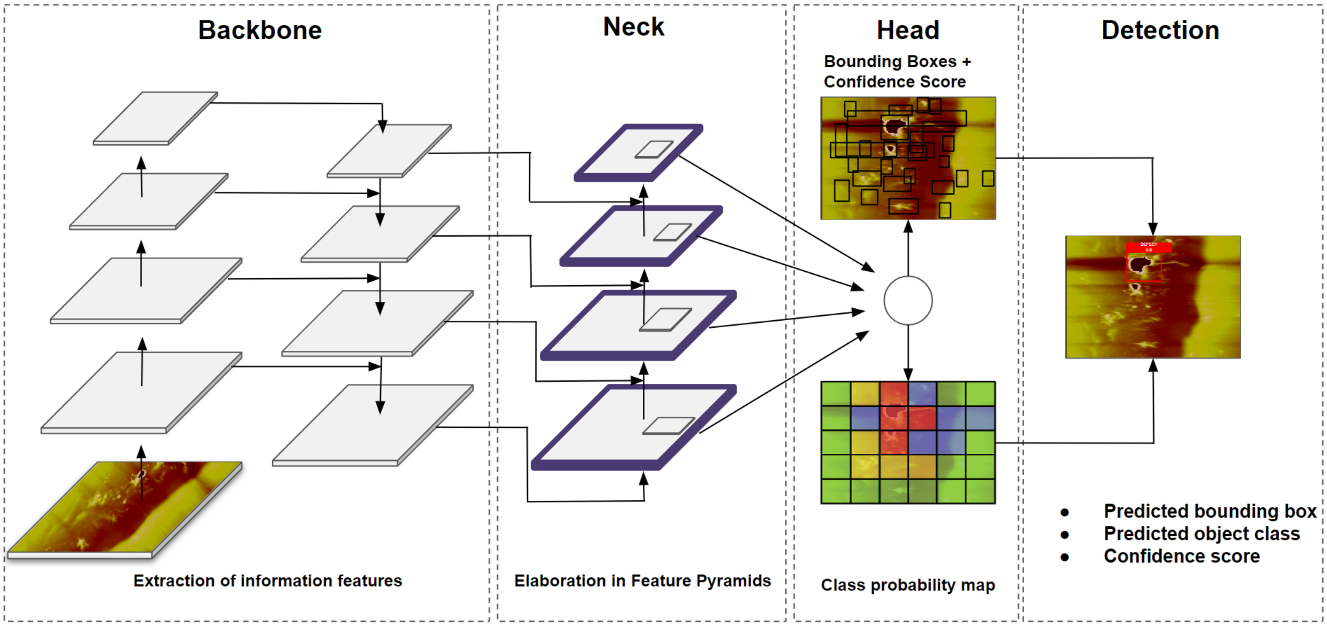

Fig. 2. Architecture of the YOLOv5 neural network.

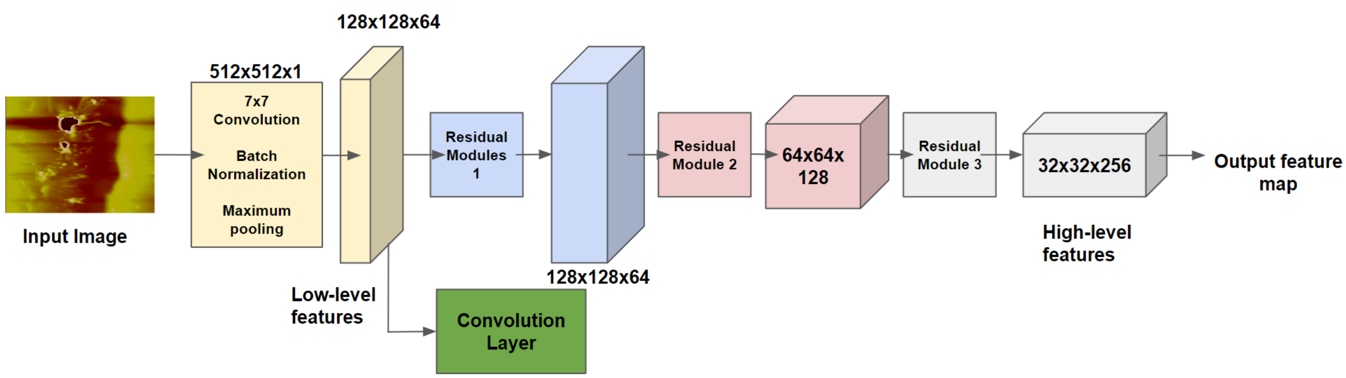

Fig. 3. Architecture of ResNet-34.

very deep neural networks without suffering from the vanishing gradient problem, a common issue in deep neural networks [14]. The core idea behind ResNet is using “residual connections”, which allows the model to learn a residual mapping between the input and output of each layer instead of trying to learn the full mapping from input to output directly. As an example, Resnet-34 [15] [16] is used in this work.

Therefore, to leverage the advantages of both YOLOv5 and ResNet-34, these two approaches seamlessly integrated together into the proposed DL network, where YOLOv5 is the “pipeline” of the defect detection involving both defect detection and localization. In particular, YOLOv5 detects the defects (blemishes) from the jpeg AFM images and identifies their locations in the images (Fig. 2), and these detected defects are then processed by the Resnet-34 for classification of the defect types. This way, the high-level features extracted and classified by ResNet-34 can be leveraged to improve the overall classification performance.

2) DL Model Training Dataset: To train the DL model, the converted jpeg images were used.

Data Annotation The phase-contrast images were generated from the jpeg files and used for defect annotation. Accurate identification of defect shapes is crucial to the success of the proposed DL network. We utilized an open-source approach called OpenLabeling [17] for data annotation. The images were annotated manually by drawing a bounding box for each defect detected by the experimental executors. Using OpenLabeling, the location and category of blemishes (i.e., defects) in each sample image were labeled (i.e., annotated). After turning off the marker, a text .txt files that contains the labeled defect information is generated. Specifically, each

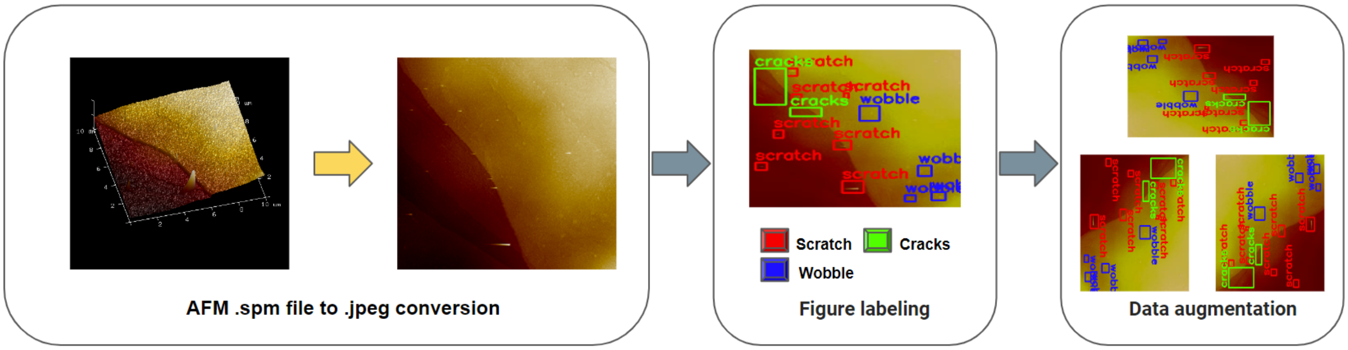

Fig. 4. Training data Preparation.

defect has three sets of parameters: object class (i.e., defect type) index, (x, y) coordinates that represents the center position of the labeled defect, and the horizontal and vertical dimension (i.e., width and height) of the defect. The location and dimension parameters are the normalized values with respect to the image size.

However, collecting sample images took a considerable amount of time and effort since the user had to manually scan the samples and capture the images. Despite our best efforts, the annotated dataset was still relatively small.

Data Augmentation To overcome the challenge of having a small dataset for training, we employed data augmentation approaches. Specifically, the annotated images mirroed, rotated, clockwise or counterclockwise by 90°, and flipped, upside-down and left-right. These operations created additional samples (with various orientations) to be added to the training set. By adding more samples, the performance of the DL network was improved and made to be more resilient to the different orientations of defect shapes observed during inference. The entire process of training data preparation is shown in Fig. 4.

C. *Training with Transfer Learning*

The prepared training set that included both defect-free and defective images samples was used for training the proposed integrated DL model. Each imperfection in the images was accurately annotated to achieve the highest possible training performance.

Pre-trained weights from a traffic light identification dataset were utilized to reduce the time cost for training and improve the performance of the network. Then transfer learning techniques were employed to fine-tune the network based on changes in accuracy.

To train the network, the dataset was split into a training set and a testing set. The training set contained 75% of the entire dataset, while the testing set contained the remaining 25%. The images were used as the input to the DL model. Note that the training set was augmented as discribed previously to further improve the performance of the network.

The network's performance was evaluated based on the loss computed after processing each image. The lost function was used to optimize the network during training, which improved its accuracy in detecting and classifying defects in AFM images.

III. Results and Discussion

AFM topography images of Highly Ordered Pyrolytic Graphite (HOPG) and hard disk surface samples were used for training and validation in this work. For each sample, 200 images were acquired initially before data augmentation.

The proposed DL-based approach was enabled to locate defects and identify its specific shapes with improved accuracy and efficiency. As the performance, this approach paved the way for automated quality control in various fields such as manufacturing, materials science, and biomedical research. During the data collection and annotation phase, we carefully annotated them with the corresponding defect shapes. The annotated datasets were then used for data augmentation, which was involved applying various transformations to the images to increase the size and diversity of the dataset.

A. *DL Model Training and Optimization*

To train the DL model, a transfer learning strategy was implemented. Specifically, the pre-trained weights as aforementioned, were used for the DL network. Then the model was trained by using the high-pixel images in the dataset before the learned weights were further refined through additional training using images with mixed resolution.

To identify the optimal neural network configuration for the proposed model, a series of tests have been conducted with different permutations of network parameters. This involved varying the training batch size, the epoch number, and optimizer type, such as Adam [18] and stochastic gradient descent (SGD) [19], for backpropagation, as well as the learning rate. We evaluated each condition by using the mean

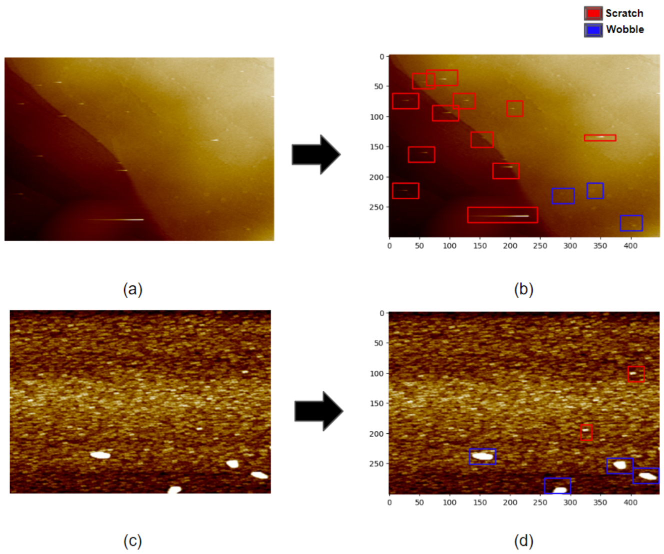

Fig. 5. Defection detection test results of the HOPG sample (a) and (b), and hardisk surface sample (c) and (d).

average precision (mAP) metric for all defect shapes, and the results of these tests are summarized in Table 1.

Based on the mAP scores, we selected the best-performing parameters that achieved the highest accuracy. The optimized model configuration is shown in the last row of Table 1. In the training progress, it is noticeable that the learning rate gradually increased to 0.001 and then decreased to 0.0002 over 500 epochs. This phenomenon indicates the over fitting issue occurred once the epoch number was more than 500.

With these optimized model configuration, the overall training and test accuracies were 89.3 % and 91.6%, respectively. The total training time was 5 min. On the contrary, directly training the model using the entire dataset did not provide similar performance: both the training and validation accuracy were less than 73%, and the training time was 6 to 9 min. Thus, the advantages of using the transfer learning technique is clear. Finally, the defect detection test results of the two aforementioned samples are shown in Fig. 5, in which each the defect types and their locations and sizes are accurately captured by the DL model.

Therefore, the performance of the proposed AI framework for AFM image defect detection and classification was demonstrated. Compared to manual blemish identification, our proposed approach offers significant time savings with high accuracy and can operate during the AFM real-time operations other than the operation in data after-process. Furthermore, the output of the framework includes the localization of the detected blemish spots. This feature can provide useful guidance for AFM imaging location selection and sample repair.

As for future work, we will explore other features of the DL network in detection and classification to further improve the performance of our approach. Moreover, the proposed framework will be extended to include features such as defect image repair, improper probe-sample interaction detection which facilitates the prompt of the probe replacement and reduces the risk of further damage to the sample.

Table 1. Performance of the DL model trained with different network configurations. The mAP value over all defect shapes is used for selecting the optimal configuration (highlited).

Optilizer	Batch	Epochs	Learning	mAP
SGD	16	1000	0.001	62.3
SGD	32	500	0.001	64.4
SGD	32	1000	0.001	66.1
SGD	16	500	0.0001	66.4
SGD	16	500	0.001	69.5
Adam	16	500	0.001	81.0
Adam	32	500	0.0001	83.4
Adam	32	1000	0.001	85.2
Adam	16	1000	0.001	86.2
Adam	32	500	0.001	90.2

IV. Conclusions

In this paper, a DL model for AFM image defect detection and classification has been proposed. The proposed DL model implements a YOLOv5 defect detector and a Resnet-34 classifier. To improve the performance of the DL model, data augmentation and a transfer learning scheme were used to overcome the challenges of defect detection using model trained with limited data size. High accuracy of the proposed AI framework was demonstrated in terms of defect detection and classification. The proposed AI approach will greatly reduce the time and labor cost in AFM images quality analysis, and has the potential to extended to other applications, such as manufacturing, material engineering, and biomedical engineering.

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