

# Towards Automated Defect Classification in Atomic-Resolution Images Via Image Augmentation

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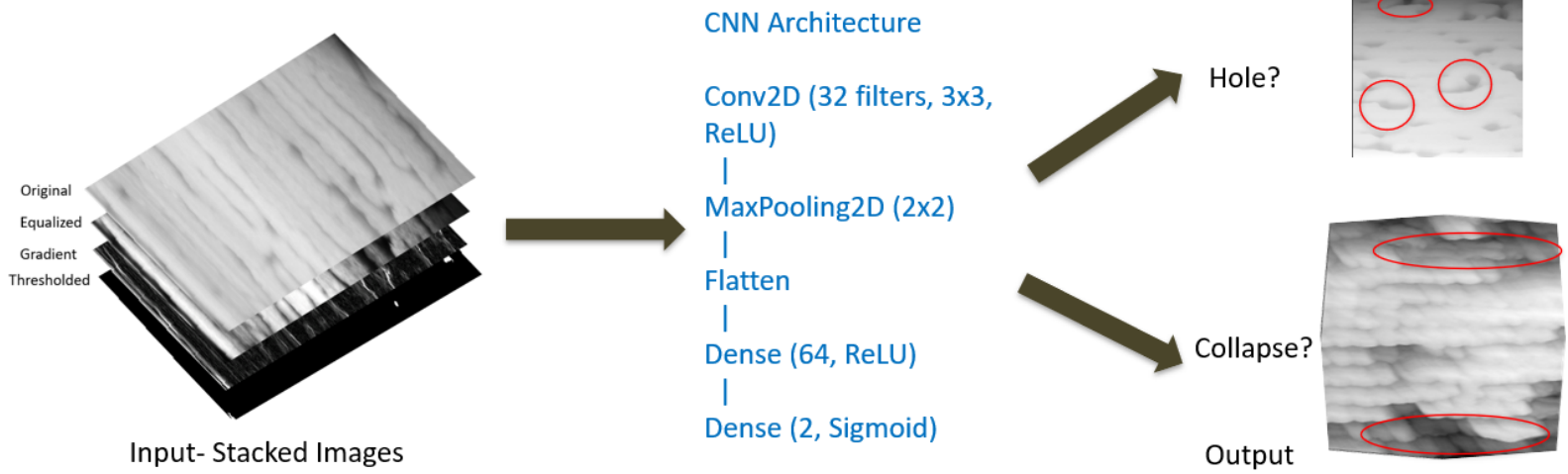
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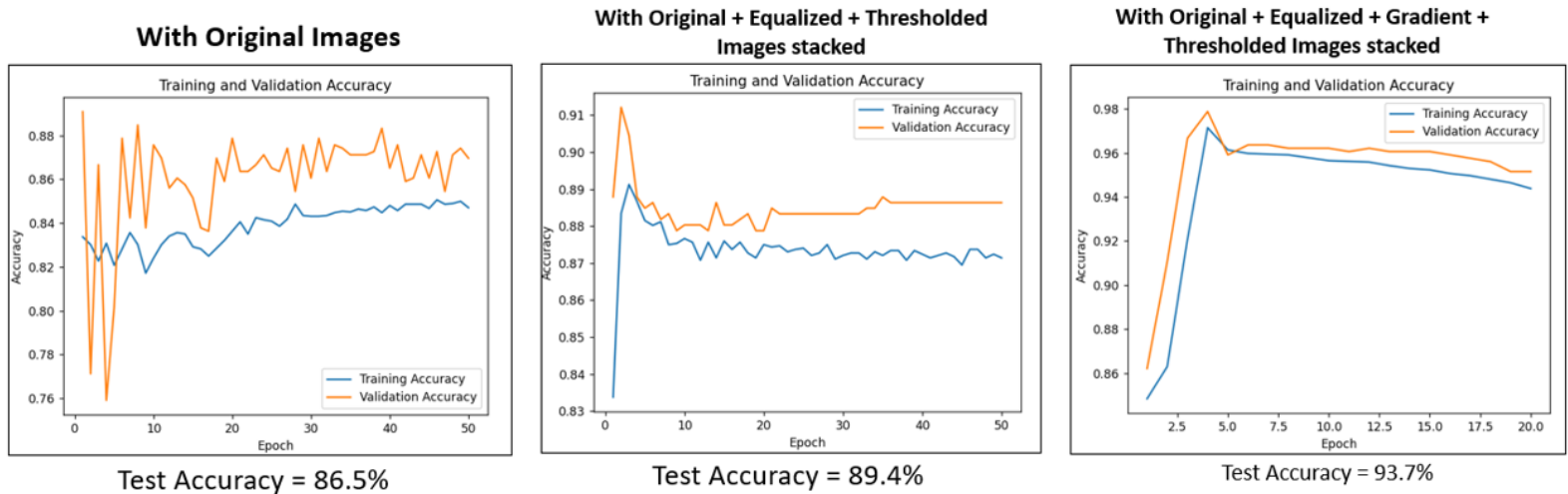
The use of nanomaterials has proved beneficial for applications ranging from improved drug delivery in healthcare, for use in anti-microbial and scratch-resistant coatings to advances in integrated circuit design. However, the widespread use of nanotechnology relies heavily on the scalability of technologies to manufacture 3-dimensional (3D) nanostructures. Real-time nanoscale metrology and closed-loop process control are crucial areas requiring innovation to enable continuous high-volume nanomanufacturing. Inline imaging of nanopatterns to detect structural flaws forms one component of overall product yield control<sup>1</sup>. This work presents the automated classification of defects in periodic nanostructures using images from an Atomic Force Microscope (AFM) with a computer vision-based approach for implementation in inline nanoscale metrology. Specifically, it relies on a new feature engineering approach that exploits image transforms (e.g., gradient to identify areas with rapid intensity variation, threshold to accentuate pixel-pixel variation, and equalization to reveal details in dark and bright regions equally) for model training. Grayscale AFM images depict 3D surface topographical information, with grayness levels indicating height values. This information is lost when applying such transforms. For this reason, the preprocessed images are used in conjunction with the original images for model training. In this application, a library of images captured on stationary samples using a modified single-chip, table-top AFM is used. Random linear geometric transformations (flips and rotations) are introduced to the original images, increasing the dataset size by a hundredfold. Each of the aforementioned image transforms is then performed on the new dataset. A Convolutional Neural Network (CNN) is trained on the augmented image dataset (comprising the original and transformed images) to identify and classify “hole” and “collapse” defect types. It is consistently observed that augmenting original images with preprocessed images enhances performance on the test data (Figure 2). Model performance can further be enhanced by tuning the CNN hyperparameters such as kernel size and the numbers of hidden layers and dense neurons. In its ultimate implementation inline in Roll-to-Roll (R2R) nanomanufacturing, we anticipate automated model training too to be feasible inline, perhaps using a moving window approach<sup>2</sup>.

## References:

1. W.-T. Chen, R. A. Chowdhury, J. Youngblood, and G. T.-C. Chiu, in 2018 Annual American Control Conference (ACC) (IEEE, 2018)
2. P. Kang, D. Kim, H.-j. Lee, S. Doh, and S. Cho, Expert Systems with Applications 38, 2508–2522 (2011), ISSN 0957-4174



**Figure 1:** Architecture of the Convolutional Neural Network used for preliminary simulations. An image is classified as having a Hole type defect if there is a local height depression in a small region, and it is classified as having a Collapse type defect if there exists a continuum of such depressions. Stacked, uniformly sized images serve as the model inputs.



**Figure 2:** Test Accuracies for three combinations of image stacking. a) Original images used in isolation result in relatively low test accuracies, b) Performance improvement observed when Equalized and Thresholded images are included, c) Best performance observed with all 4 images used in conjunction (# Epochs = 20 due to compute power limitations)