DEEP LEARNING APPLICATION FOR AUTOMATED CLASSIFICATION OF PARTICLE MORPHOLOGY IN ROOT CAUSE ANALYSIS

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ABSTRACT

In the realm of failure analysis, accurate identification of the particle morphology is critical to determine the source of contamination on hard disk drives (HDDs). The size and shape of the particle demonstrates the characteristics and properties of material in microscopic level. However, manual classification of shape demands human effort making it susceptible to inaccuracies and requires substantial time.

This technical paper utilized deep learning methods, particularly convolutional neural networks (CNNs) on existing microscopic imaging database from scanning electron microscopy (SEM) to create a generalized model to accurately identify particle morphology.

The implementation of Residual Network 50 (ResNet-50) architecture facilitates the classification of ten distinct morphological shapes. After processing the training, validation, and test set; Particle Morphology Auto-Classifier (PMAC) application achieved the target by exceeding 90% accuracy rate for Bead, Beads, Droplet, Flat, Tube, 88-89% accuracy for Soft and Clustered, and 70-75% for Grain, Irregular, and Fiber.

1.0 INTRODUCTION

Artificial intelligence (AI) is the utilization of modern technological advancements to develop machines and computers that can mimic a human brain or perform cognitive functions such as processing visual information, responding to spoken or written language, reasoning, and data analyzation [1]. Machine learning (ML) is a branch of artificial intelligence that allows the computer system to identify patterns in a big data set. Presently, this technique is applied in the field of material science [2].

Deep learning (DL) is a subset of ML that can analyze big data set to create an accurate predictive model. DL algorithms and models such as Convolutional Neural Networks (CNN) and Recurrent Neural Networks (RNN) have demonstrated remarkable capabilities in terms of image recognition and pattern detection. Thus, it can be used to identify the shape, size, and other properties of a particle with high precision and accuracy [3]. This approach is ideal for understanding particle images from spectroscopy and microscopy methods. The creation of these AI-driven methods automates particle morphology identification, minimizing bias and accelerating the analysis process. Figure 1 demonstrates the relationship between AI, ML, and DL and their development through the years.

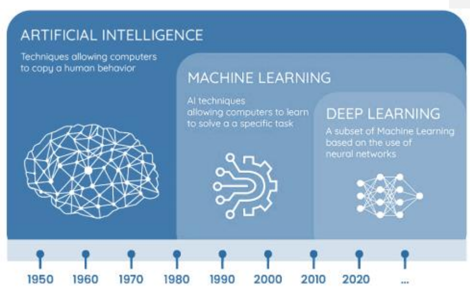


Figure 1. Relationship of AI, ML, DL [4].

ResNet is a commonly used CNN architecture that yields high accuracy compared to other architectures; namely, AlexNet and GoogLeNet. It is a type of deep convolutional neural network that specializes in image classification and object detection. It was founded by Microsoft researchers; namely, Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. It became a successful CNN architecture by winning the ImageNet Large Scale Visual Recognition Challenge (ILSVRC) in 2015 surpassing the general human error rate of 5% via achieving an error rate of only 3.57% [5]. ResNet architecture comes in various depths depending on the number of layers, such as ResNet-18, ResNet-34, and ResNet-50. It enhances the training of more neural layers while minimizing the error rate [6,7]. The concept of ResNet will be created or applied on the software application called "Microsoft VSCode" and using "Python" as the programming language. Additionally, creation of PMAC also used "Tensorflow," which is an open-source machine learning library or framework that allows "Keras," an application programming interface (API), to build high-level neural network [8]. Collectively, they form a robust ecosystem for training and developing machine learning models.

When dealing with AI-driven technologies, data is usually divided into three sets: training, validation, and test set shown on Figure 2. The training set is used to train the network, this is where the model learns the pattern of the data. Validation set is used to evaluate the performance of the model. The result from the validation set is used to tune the hyperparameters to develop the model. The test set is used to evaluate the performance of the final model [9,10].

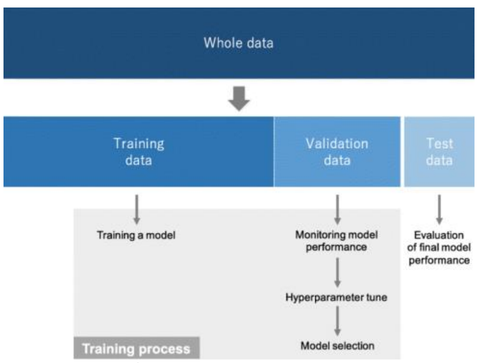


Figure 2. Division of Data [10].

Using the advanced concepts of AI, engineers of Toshiba Yokohama, Japan developed an AI software called "PMAC." This software aims to accurately identify the morphology of a contaminant based on its SEM image. Previously, classification of images by morphology is manually judged by engineers which is prone to human error and time-consuming.

The shape of a contaminant is essential to the investigation of HDD failure in terms of narrowing down the possible root-cause of the failure. The shape information along with other characteristics of the contaminant, such as the elemental composition, can be compared with a pre-determined contaminant database to generate a list of possible sources of failure (e.g., drive parts, environment, process-derived, etc.). Moreover, like in any AI software, the performance of PMAC highly depends on its training or learning process. Its accuracy is said to increase proportionally to the number of the training images.

In this paper, 7,125 images were collected and used to train, validate, and test the PMAC software—with ResNet50 as the DL model and Keras as the library base. The correct answer ratio per label, classification accuracy (based on the PMAC judgment performance) and generalization performance of the whole data will all be measured. The resulting values shows the overall judgment accuracy of PMAC. This study aims to increase the prediction accuracy PMAC from previous 84% accuracy.

2.0 REVIEW OF RELATED WORK

2.1 AI-enabled materials research

With AI technology, scientists were able to accelerate novel materials discovery due to enhancement of hypothesis testing and data analysis from experimentation. Aside from discovery of new materials, researchers were also able to design material by examining crystal structure and chemical composition based on existing data with the help of deep learning algorithms [10]. A study by Dahy et al. (2023), utilized 750 images of Palladium nanoparticle to classify its particle type (i.e., lines, intersections, networks, ellipses, and circles). The team used Visual Geometry Group 19 (VGG-19) as their deep neural network for feature extraction and classification of images. The promising model showed a 97% accuracy rate which indicated an excellent performance of the nanoparticle classifier from SEM images [11]. Today, AI has been widely used by different field of study to create breakthrough innovations for the benefit of the world.

2.2 Challenges of Deep Learning

While deep learning is a powerful tool in the field of AI, there is still a need of continuous research and development to address its challenges. One of the most common challenges of deep learning is the overfitting of data. The purpose of deep learning is to create a model that can generalize the characteristics of the data; however, overfitting occurs when the model adapts closely to the training set [12]. Overfitting is a situation where the model memorizes the statistical noise instead of learning the patterns of the data. Hence, the model tends to perform less when applied to a new dataset. To check if the model is overfitted, validation and test set evaluates the performance of the trained model by monitoring and comparing the loss and accuracy of training and validation set. If the model performs well on the training set compared to validation set, then the model is overfitted [10]. For the past years, ML engineers were able to develop methods on how to minimize overfitting in ML. Data augmentation, shown in Figure 4, is one of the common ways to reduce overfitting of image dependent model. It is a technique of creating new images from the original image by flipping, rotating, cropping, adjusting contrast and brightness of the image, which is applied to PMAC software. With this technique, the model will increase the generalization ability of the model [13].

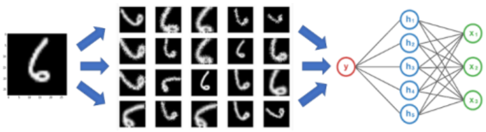


Figure 4. Example of Data Augmentation [14].

3.0 METHODOLOGY

The methodology employed in this study encompasses a structured approach, beginning with image acquisition followed by meticulous image sorting. Subsequently, the study proceeds with PMAC Model Training and Data Augmentation. Finally, the study culminates in the interpretation of the results, wherein the outputs of the model are analyzed and evaluated.

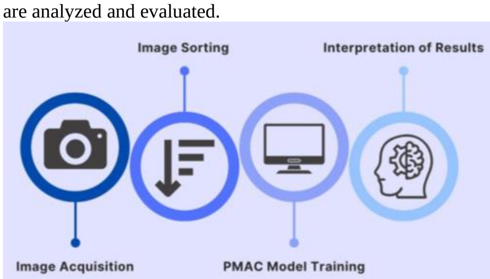


Figure 5. Overall Process Flowchart

3.1 Image Acquisition

A total number of 7, 125 images were collected—with the total number of images for each of the 10 shape classifications (morphology) shown in Figure 6. Overall data was then split into three sets: training, validation, and test.

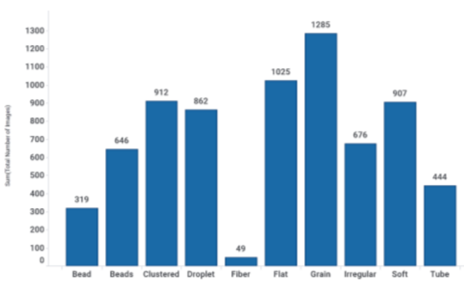


Figure 6. Number of Images per Manual Classification

3.2 Image Sorting

The training set is comprised of 70% of all the collected images, whereas the validation and test sets are both at 15%. These percentages, along with their corresponding actual values, are demonstrated in Figure 7.

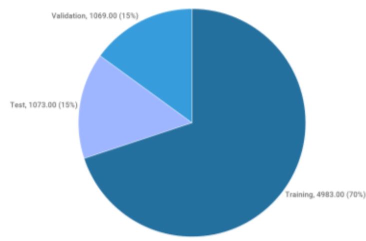


Figure 7. Image Distribution per Set

3.3 PMAC Model Training

Furthermore, Figure 8 shows sample SEM images collected per shape classification. These images are fed to the PMAC software during its training. Support engineers in Toshiba Yokohama performed the model training using a PC specially purchased for this purpose. This machine learning hardware utilizes Tensorflow + Keras base as its machine learning library and ResNet50 as the learning model. Data augmentation was also performed to reduce overfitting thus, increase PMAC's generalization ability.

Commented [rpnFAD1]: Consistency as shape classification not "type"

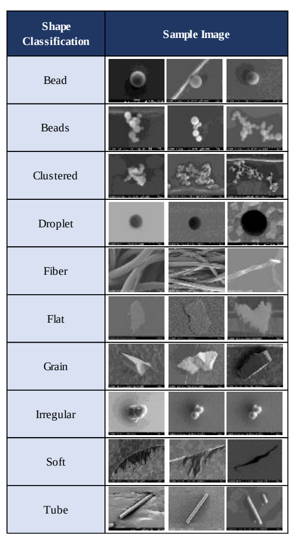


Figure 8. Sample SEM Images per Shape Classification

3.4 Interpretation of Results

Training the PMAC software generates an accuracy plot, a loss plot, and a confusion matrix. These three serves as basis of how successful the training was (i.e., AI performance) and the accuracy of PMAC in judging the correct morphology per image input.

4.0 RESULTS AND DISCUSSION

4.1 Overall Accuracy Plot

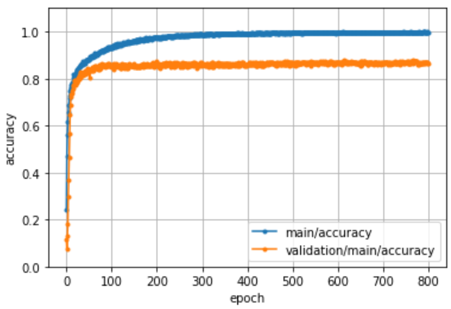


Figure 9. Overall Accuracy Plot

Validation accuracy measures the performance of the correctly classified images that the model hasn't seen during training process. It shows the performance of the model in generalizing new and unseen data. The classification accuracy plot generated after the model training is shown in Figure 9. It indicates the accuracy of both the training data (main/accuracy) and the validation data (validation/main/accuracy) in determining the correct contamination morphology per image, and the corresponding epoch number. An epoch represents the number of times the data is fed to the neural network. By repeatedly training the data, it can improve the weights. Based on the figure, the overall classification accuracy for the training data and the validation data approaches 100% and 87%, respectively, as the epoch number increases.

4.2 Overall Loss Plot

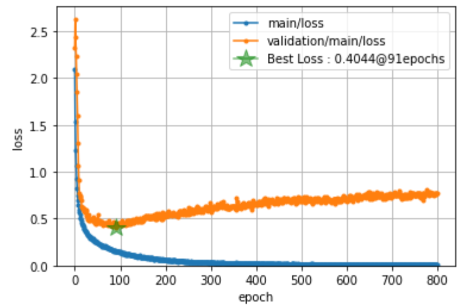
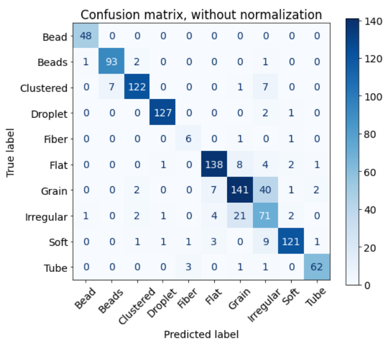


Figure 10. Overall Loss Plot

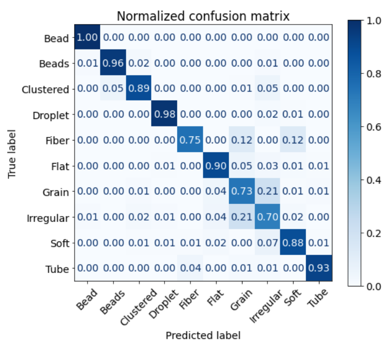
Loss can be described as the difference between the true value and predicted value by the model. The larger the loss, the larger the errors committed by the model on the data. A loss plot was also generated after the training process as shown in Figure 10. It can be observed that the error for the shape determination by the training data (main/loss) approaches 0 at epoch numbers above 500. On the other hand, the validation data (validation/main/loss) continued to increase after 100 epochs and began to show indication of stabilization at above 600 epochs—with the best loss achieved at 91 epochs. The graph shows that the training set performed better than the validation set, which demonstrates the presence of overfitting.

4.3 Confusion Matrix

In machine learning, confusion matrix is used to summarize the performance of the model from the test set. It displays the number of accurate and inaccurate prediction of the model. The classification accuracy per morphology type is given in Figure 11. This figure presents the results of the morphology determination by the network model using the chosen test data as a pair of the correct label input into the model (True Label) and the corresponding judgment label output by the model (Predicted Label). Normalization was also done to generalize the accuracy rate for all morphology classifications, since the number of correct predictions per shape type varies on their corresponding test data amount.



(a)



(b)

Figure 11. Confusion Matrix for 23B: (a) Actual (values are by number of images) and (b) Normalized (values are by rate)

To understand Figure 11, Grain as an example, 73% is predicted by PMAC as Grain, while 21% was misclassified as Irregular, 1% as Soft, 1% as Tube, 1% as Clustered, and 4% as Flat.

Moreover, it can be derived from Figure 11 that there are several misclassified images even for morphology types with high accuracy rate (i.e., 90% and above). This can be attributed to two things. The first being that a limitation of PMAC is its low ability to correctly classify morphology from images containing a combination of particles with varying shapes. Second is in ensuring that training images (which are initially manually judged via the naked eye) are fed to the model under their correct morphology classification. For instance, some irregular particles were fed to the model as grain particles instead and vice versa (which is reflected in Figure 11 with about 21% of the morphology type being misclassified as the other). Thus, creating further confusion during PMAC's judging process and decreasing the accuracy rate of certain morphology types.

5.0 CONCLUSION

Upon completion of the training, validation, and testing procedures, the validation set yielded an accuracy rate of 87%. Subsequently, during evaluation on the test set, the PMAC application surpassed the predefined performance threshold, achieving an accuracy rate exceeding 90% for five of the ten morphology types. Specifically, these classifications include Bead (100%), Beads (96%), Droplet (98%), Flat (90%), and Tube (93%). Additionally, two out 10 morphology types achieved an accuracy rate for Soft (88%) and Clustered (89%). Nevertheless, it is noteworthy that the PMAC application demonstrated comparatively lower accuracy rates for three morphology types, namely Grain (73%), Irregular (70%), and Fiber (75%). Potential attributions for this shortfall may include constraints from the quality of manually classified training images and instances of misclassification within the dataset.

6.0 RECOMMENDATIONS

To enhance the performance of the current deep learning model and image classification system, our team suggests four key improvements. First is to gather and increase the number of training images, especially for Fiber, to build a more versatile model and to accurately classify wider range of particle shape. Second is to improve PMAC's ability to recognize combination of different shapes in a single image, as this is the current limitation of the model. Third is to review the manually classified images such that it will no longer misclassify Irregular, Grain, and Flat particles. Finally, it would be beneficial to leverage on alternative CNN architecture beyond the current framework to maximize the potential or uncover new strategies to enhance the performance of the model. By pursuing these recommendations, it can significantly enhance the reliability and robustness of PMAC in root cause analysis and contamination source identification tasks.

7.0 ACKNOWLEDGMENT

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8.0 REFERENCES

1. AI vs. Machine Learning: How Do They Differ? | Google Cloud. (n.d.). Google Cloud.

https://cloud.google.com/learn/artificial-intelligence-vs-machine-learning

2. IBM data and AI team. (2023, July 11). AI vs. Machine Learning vs. Deep Learning vs. Neural Networks: What's the difference? IBM Blog. https://www.ibm.com/blog/ai-vs-machine-learning-vs-deep-learning-vs-neural-networks/
3. Ahmad, J., Farman, H., & Jan, Z. (2018). Deep learning methods and applications. In SpringerBriefs in computer science (pp. 31–42). https://doi.org/10.1007/978-981-13-3459-7_3
4. The difference between AI, Deep Learning, Machine Learning in agriculture. (n.d.). https://www.dilepix.com/en/blog/difference-artificial-intelligence-deep-learning-agriculture
5. He, K., Zhang, X., Ren, S., & Sun, J. (2015). Deep residual learning for image recognition. arXiv (Cornell University). https://doi.org/10.48550/arxiv.1512.03385
6. Banjara, B. (2023, February 7). Deep residual learning for image recognition (RESNet explained). Analytics Vidhya. https://www.analyticsvidhya.com/blog/2023/02/deep-residual-learning-for-image-recognition-resnet-explained/
7. Boesch, G. (2024, March 12). Deep Residual Networks (RESNet, RESNet50) – 2024 Guide. viso.ai. https://viso.ai/deep-learning/resnet-residual-neural-network/
8. Introduction to TensorFlow. (n.d.). TensorFlow. https://www.tensorflow.org/learn
9. Shah, T. (2021, May 24). About train, validation and test sets in machine learning. Medium.https://towardsdatascience.com/train-validation-and-test-sets-72cb40cba9e7
10. Yamashita, R., Nishio, M., Gian, R. K., & Togashi, K. (2018). Convolutional neural networks: an overview and application in radiology. Insights Into Imaging, 9(4), 611–629. https://doi.org/10.1007/s13244-018-0639-9
11. Dahy, G., Soliman, M., Alshater, H., Słowik, A., & Hassanien, A. E. (2023). Optimized deep networks for the classification of nanoparticles in scanning electron microscopy imaging. Computational Materials Science, 223, 112135. https://doi.org/10.1016/j.commatsci.2023.112135
12. Awan, A. A. (2023, August 24). What is Overfitting? https://www.datacamp.com/blog/what-is-overfitting
13. Dilmegani, C. (2024, December 26). What is Data Augmentation? Techniques & Examples in 2024. AIMultiple: High Tech Use Cases &Amp; Tools to Grow Your Business. https://research.aimultiple.com/data-augmentation/
14. Data Augmentation: How to use Deep Learning when you have Limited Data - KDnuggets. (n.d.). KDnuggets. https://www.kdnuggets.com/2018/05/data-augmentation-deep-learning-limited-data.html

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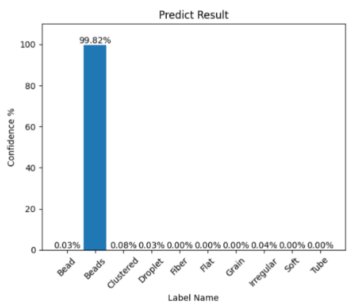
10.0 APPENDIX

Appendix A – PMAC Interface with Predicted Result



Appendix B – Distribution of Images per Set

Shape Classification	Number of Training Images	Number of Validation Images	Number of Test Images
Bead	223	48	48
Beads	452	97	97
Clustered	638	137	137
Droplet	603	129	130
Fiber	34	7	8
Flat	717	154	154
Grain	899	193	193
Irregular	473	101	102
Soft	634	136	137
Tube	310	67	67
Total	4983	1069	1073

Appendix C – Accuracy Plot from previous training (84%)