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ARTIFICIAL INTELLIGENCE IN METALLOGRAPHY
VEŠTAČKA INTELIGENCIJA U METALOGRAFIJI

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Keywords
• artificial intelligence
• quantitative image analysis
• AI based prediction
• crack propagation prediction
• problem identification

Abstract

Integrating artificial intelligence into various manufacturing and quality control processes is extremely popular these days and widely implemented by different companies in the field of automotive, aviation, industry manufacturing as well as pharmaceutical industry. Significantly, the integration of artificial intelligence into material science fields such as metallography and quantitative image analysis techniques has been pivotal in analysing and understanding the microconstituents and microstructures of different metals. Deep learning-based methods for image analysis and segmentation are employed to allocate semantic tags on every pixel of the image and therefore dividing the image into more detailed sections. However, this process is not that simple as it seems at first, since several parameters can be critical in terms of effectiveness. For example, such parameters are the choice of the learning method, as well as the reliability of thousands of already processed image-based information that form the basis of the procedure. Perhaps one of the huge tasks is collecting and organising the right amount of processed image information. This article is about presenting the complexity of the topic, highlighting various learning methods employed in enhancing the AI developed models and the set of information that is essential for providing usable end results, that can be integrated into the process of metallographic and quantitative image analysis.

Ključne reči
• veštačka inteligencija (AI)
• kvantitativna analiza slika
• predviđanje zasnovano na AI
• predviđanje širenja prsline
• identifikacija problema

Izvod

Integracija veštačke inteligencije u različite proizvodne i procese kontrole kvaliteta danas je izuzetno popularna i široko primenjena od strane različitih kompanija u oblastima automobilske industrije, avijacije, industrijske proizvodnje, kao i farmaceutske industrije. Značajna je integracija veštačke inteligencije i u oblastima nauke o materijalima, kao što su metalografija i tehnike kvantitativne analize slike, gde je od ključnog značaja za analizu i razumevanje mikrokonstituenata i mikrostruktura različitih metala. Metode zasnovane na dubokom učenju za analizu i segmentaciju analize slika koriste se za dodeljivanje semantičkih oznaka svakom pikselu slike, čime se slika deli na detaljnije sekcije. Međutim, ovaj postupak nije tako jednostavan kako se na prvi pogled čini, jer pojedini parametri mogu biti ključni u pogledu efikasnosti. Na primer, takvi parametri su izbor metode učenja, kao i pouzdanost hiljade već obrađenih informacija zasnovanih na slikama koje čine osnovu postupka. Verovatno je jedan od najvećih zadataka prikupljanje i organizovanje odgovarajuće količine obrađenih informacija o slikama. U ovom radu se bavimo predstavljanjem složenosti teme, isticanjem raznih metoda učenja, koje se koriste za unapređenje razvijenih AI modela i skupa informacija koji je neophodan za pružanje upotrebljivih konačnih rezultata, koji se mogu integrisati u postupak metalografske i kvantitativne analize slike.

INTRODUCTION

There have been developments and advancements in machine and deep learning models and the introduction of new equipment in scientific fields that play a crucial role to accelerate material analysis and research in general. Various models such as *Diffusion models* in computer vision which are applied to applications such as *Microsoft Bing Image Creator* to get rid of structure in data distribution with an onward process and replace the destroyed structure in data with help of a tractable model in a reverse process, /1/. The most frequent question that arises among most material scientists amidst AI development and advancements is whether this approach can effectively learn and subsequently be applied in metallographic and quantitative image analysis of materials, especially metals with desired properties, /1, 2/.

For a long period, physics-based techniques, including finite element method (FEM) analysis which are relatively expensive and require application of known physical relationships have been employed in material microstructural analysis. Recently, due to technological advancements, material science has blended in the use of machine learning techniques in material properties characterisation and prediction. One of the challenges faced by physics-based techniques is the fact that it is difficult to deal with complex materials and the nature of the microstructure. Machine learning (ML) generative models have played a successful role in analysing complex relationships like mechanical properties without the direct knowledge of the basic physics, therefore helping in fast analysis of material's microstructure. In contrary, metallography, which is an important aspect of material science is likely to strengthen due to the advancement of machine learning models, /2, 3/.

The primary importance of AI in material science is to aid experts in this field by providing them with AI powered equipment to magnify their decision-making abilities when performing various research and analysis related to this field. The application of AI in material science has increased over years, now especially in the analysis of material microstructure such as grains, inclusions, defects and grain boundaries. The term microstructure can be defined as the organisation of phases and defects in a metal or material on a micrometre or centimetre length scale, /4/. It is easy to determine mechanical and physical properties such as hardness, toughness, ductility, brittleness and other properties of materials if their microstructure is understood. Therefore, through analysing the metallographic and quantitative images of materials (especially metals) the structure, quality and morphology of these materials can be understood and made easy to categorise them for different engineering and industrial applications. In this article, various image analysis models are outlined highlighting their crucial role in metallography. Deep learning models include U-Net models which a convolutional neural network (CNN) based model helps in image segmentation, usually by assigning semantic tags to each pixel of the image. Through image segmentation, different items in a metallographic structure such as inclusions, grains and defects can be categorised by assigning different tags to each pixel of the specific image. These models can accurately partition and identify various microstructural characteristics in materials. This reduces human labour relatively shortening the analysis and characterisation process. The CNN is made up of two parts, namely, the encoder and decoder. The encoder is also called the contraction path and is responsible in trapping contextual information of the input image. It slowly reduces the dimensions of captured images and maximises the number of feature channels. The decoder is referred to as the expansion path, and it provides accurate localisation using transferred convolution sections which up sample the feature map. The data outputs from the encoder are combined with the feature map from the corresponding decoder path layers through skip connections. These skip connections are important as they give detailed high-resolution information, /5, 6/.

Machine learning (ML) models such as the Generative Adversarial Network (GAN), Denoising Diffusion Probabilistic Models (DDPM) and the Variational Autoencoder (VAE) have been developed to produce microstructure images, /1/. Conditional based generative models have been used to synthesize images for high-carbon steels. There have been several performance improvements of these models, especially the GAN-based model which developed some mode collapse and training instability. These areas still require some improvements and therefore attract researchers to figure out better alternatives. The GAN-based models produce few outputs compared to the input data distribution, making it a less reliable model. Another issue facing the GAN-based models is the generation of blur and less detailed outputs relative to input data. This is more common in VAE and is attributed to modelling of high dimension data size to a lower latent size in the entire process, /2, 3/. In 2020, DDPM was developed in the field of computer vision, replacing GAN and VAE, therefore transforming the generation of high-resolution images. Researchers like Lee and Yun developed a DDPM model to produce images with same quality as those in a dataset with several microstructures, such as ceramics, carbonate, fibre composite, and others, /1/.

CONCEPTION AND BACKGROUND

Overall, AI-based approaches are well suited for multivariate, data-driven evaluation of microstructural characteristics, residual stresses, and data obtained from mechanical, fracture mechanics, and fatigue tests, which can only be achieved to a limited extent using conventional methods. When measuring residual stresses, AI enables the coordinated processing of data obtained using different measurement methods (HDM, XRD, MAG), the correlation of measurement results with different spatial resolutions and sensitivities, and the reliable identification of local stress peaks. In the case of microstructural analysis, AI-based image analysis is capable of automatically separating the different microstructure elements, as well as objectively and reproducibly evaluating grain size changes, phase ratios, and structural inhomogeneities. In the processing of mechanical test results - especially hardness measurements, tensile tests, and Charpy tests, AI contributes to the statistical evaluation of measurement data, the spatial mapping of local material property changes, and exploration of correlations between microstructural condition and mechanical response. In fracture mechanics and fatigue crack propagation tests, AI supports the objective identification of crack initiation and propagation characteristics, the reliable determination of critical parameters (e.g., fracture toughness, crack propagation rate).

This article presents the complexity of metallography and quantitative image analysis topics and highlights different learning methods implemented to enhance the developed machine and deep learning models. Suggestions are provided regarding the DL models for acquiring usable end results and therefore simplify the integration of AI into metallographic and quantitative image analysis and the sustainable knowledge base.

Metallography

This field of metallography is pioneered by the English scientist Henry Clifton Sorby in the 19th century. He was a microscopist and a geologist who introduced the study of microscopic structures and later discovered that properties of metals and alloys could be related to microstructure constituents such as grains and inclusions, /7/. Concepts regarding metallography are as follows.

- Experience and knowledge-based failure detection.
- Evaluation of microstructure and properties of materials. These properties include mechanical strength, toughness, brittleness, hardness and other properties.
- Determination of product reliability and failure of the material.
- Essential for designing better products by providing insights into how materials (metals) behave under different conditions.

- Ensuring better quality standards through identification of defects in materials before their application.

Quantitative image analysis

It simply means the extraction of objective and quantitative information from images applied in various fields. It includes the application of advanced algorithms and statistical techniques to analyse and measure properties and features of images. Researchers can effectively and accurately quantify aspects such as shapes, intensities and textures with an image providing valuable insights into basic data. Conceptual approach of quantitative image analysis involve:
- AI integration (support and decision making);
- image measurement and interpretation of analysis results;
- strain intensity quantification and provision of accurate measurements, /8/.

LEARNING METHODS OF AI

Learning can be defined as a continuous process of acquiring new skills, knowledge, values and preferences. In a simpler way, learning can be defined as the adaptive intelligence alteration in response to experience. Machine learning is similar to cognitive learning which is related to humans. Machines review the existing stored data and learn from it.

Machine learning is therefore a branch of AI and computer science that involves the use of data and algorithms to follow the learning processes as humans do. Machine learning is widely known for its potential in predictions from a large dataset which is far beyond human processing power. This ability attracts experts in various fields such as (manufacture, aviation, material science, transportation, etc.) to employ ML as the fundamental technology for most of their IT transformation strategies. The machine learning models learn through supervised and unsupervised learning methods depending on the data input, data type, etc. Machine learning comprises of data sets, algorithms, feature extraction, training and models.

In a supervised machine learning method, the machine solves the problem based on data that is fed to them through data sets. This is different from unsupervised machine learning method where machines learn on their own without any guided data by discovering information, creating patterns and then labelling the data, /8/. Popular machine learning (AI) techniques are given as follows.

Deep learning for Image segmentation

Deep learning involves U-Net, DeeplabV3+ and Mask R-CNN models which are commonly used for segmenting different regions in micrographs (e.g., grains, phases, inclusions and defects). This technology aids the machine to imitate the human brain and it plays a crucial role in various fields, such as image classification, voice recognition, and computer vision.

Neural networks

These are biological related programming patterns that facilitate a machine to continue learning from observational data since it is an unsupervised machine learning technique. Neural networks can be classified into different types that can be trained using this technique: Convolutional Neural Network (CNN), Recurrent Neural Network (RNN) and Artificial Neural Network (ANN). In this article, we recommend the use of CNNs for task classification to identify material types, defects or phase boundaries based on image features. These neural network-based techniques may operate in supervised or unsupervised learning frameworks, and the major drawback is that a lot of data and computational power is required for their proper functionality and learning facilitation.

Transfer learning

In this ML technique, the already trained data set is reused again to perform a new task which is similar to the already done task. The ML algorithm can learn and quickly adapt to the new task. This is possible since a data set is trained for a task and a fraction of the trained layers is transferred and combined with layers of a new data set. Transfer learning is considered less expensive since it needs less data to be trained. In addition, with an already existing data set, there is enough tagged data that can aid the accomplishment of new tasks. Pretrained models (such as VGG of ResNet) which contain general image data sets can be used by fine tuning them for metallographic image analysis, /8-10/.

APPLIED LEARNING METHOD

Given the scarcity of specialised metallographic data sets, the distinctive approach would be to use a transfer learning strategy. In transfer learning technique, the steps below can be implemented to select and train the equitable model for better end results:
Step 1: select the pretrained model like VGG, ResNet or U-Net based on your preferences. Most of the models have learned the robust feature representations from a wide general purpose data set (like ImageNet, MetalDam or COCO).
Step 2: fine-tune the model based on the metallographic data set. This will involve modifying the final layers to suit the classes present in the data set (e.g., types of phases, defects, grains, etc.).
Step 3: Training the modified model on the collected and accurately tagged metallographic images, /8/.

DATA COLLECTION AND SCIENTIFIC FOUNDATION

This section is about the description of the proposed data collection techniques in details and also the description of the collection and preparation stages of data which facilitate the teaching of AI models.

The collection of various microscopic images from known data sets (like MetalDam, COCO, etc.) or physically gathering the images from different metal specimens (like steels, cast iron, etc.) using scanning electron microscopy.

The collected images can be accurately labelled by simply resizing them in accordance with the standard format and indicating visible markings on detected defects (like cracks, porosity, etc.). However, software (like ANSYS, FEMAP, etc.) can be employed to analyse the complex images and obtain images for training the AI models.

Perform several evaluations of the collected images and employ the transfer learning technique following the previous outlined steps to ease the AI integration. Samples of images from ANSYS and SEM are shown in Fig. 1.

a)

b)

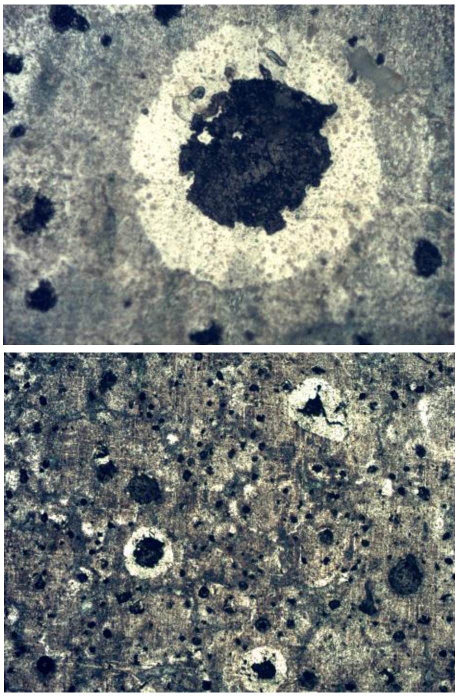

Figure 1. Engine crankshaft analysis with: a) ANSYS; b) SEM metallography.

DATA MANAGEMENT

To ensure smooth data flow, the collected data should be managed in a well-structured manner. In this structure, different steps are shown elaborating the performed tasks under each step for a better AI integration design, Fig. 2.

SOLUTION AND ACCURACY

In this section, we outline various methods and strategies that convey key aspects related to the functionality of the model. Machine learning engineers should focus on:

- improving the accuracy and effectiveness of the model by levelling up its predictive accuracy, minimising errors and ensuring proper adaption to the new data;
- elevating the operational efficiency of the model by speeding up its data processing ability while focusing on low costs and lessen the computational requirements.

To the best of our knowledge, we can conclude that the implementations of the above procedures will enable the AI models to become more powerful, adaptable and aligned with specific organisational objectives. However, there are more metrics which will help in the accuracy improvement of the AI model. These metrics aim at improving pixel-wise accuracy, precision, recall and F1 score for defect detection.

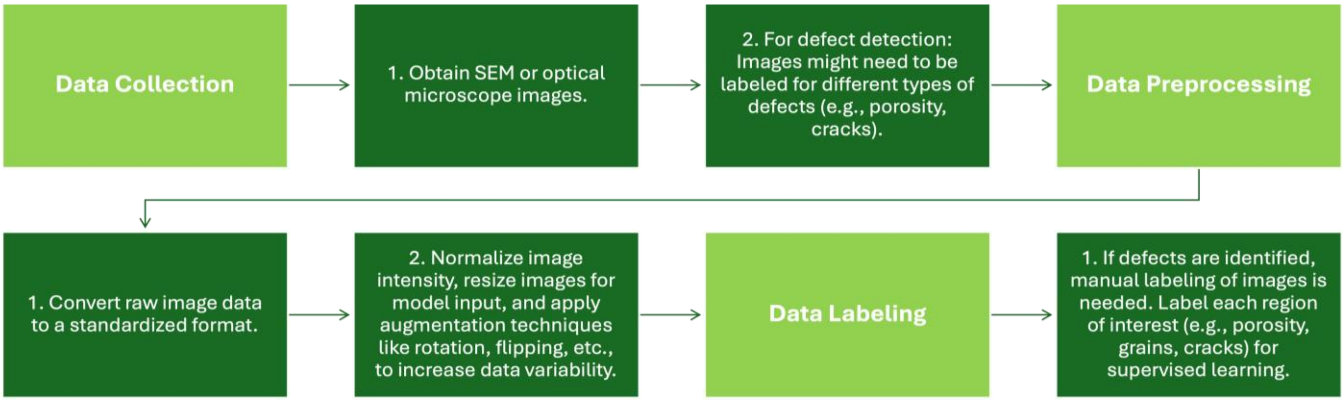

Figure 2. Structured data flow, /8/.

Class imbalance

Defects like porosity may be underrepresented. Apply more accurate techniques (like oversampling, data augmentation or weighted loss functions) to address this issue.

Overfitting

Regularisation methods (like dropout or early stopping) and data augmentation help to prevent overfitting. Cross-validation methods (like K-Fold Cross-Validation) help identify overfitting of the model where the model is evaluated based on different subsets of data, therefore minimising the chances of training a model that is biased.

Data augmentation

Techniques like SMOTE can be used for imbalanced data sets. Also, data augmentation involves producing additional data by employing transformations such as flipping and cropping for image data. Augmentation increases the ability of the model relative to variations in real world data.

Data cleaning and interpretability

Data fed to the model must be cleaned first before feeding it to the model to get rid of errors and duplicates that can lead to bias. Employ techniques like Grad-CAM for visualising which areas of the image the model should focus on.

Fine-tune hyperparameters

The model learning process is controlled by this metric. Learning processes (like activation functions, learning rates and batch sizes) are controlled by hyperparameters and therefore, accurate tuning the hyperparameters can adequately improve the model accuracy. Different methods (like Grid search, Bayesian Optimisation, etc.) can be used to achieve better model accuracy. Bayesian optimisation finds the optimal hyperparameters set using probabilistic models through modelling the function that directs hyperparameters to higher performance. This is considered to be a more efficient method than Grid search.

Model complexity

Various methods can be employed to increase the model complexity to perform the tasks which need higher accuracy end results. These methods include deepening and widening the model which add more layers or parameters to the model to improve its ability to learn more complex patterns.

Monitoring and retraining the models

Since AI models perform a lot of work it is likely that they can experience degradation in performance over time due to several factors. Therefore, frequent monitoring the model performance and retraining it with new data is very essential to ensure the model remains updated and accurate. Model drift should be performed to detect when model accuracy starts to degrade. It can be done by tracing metrics (like precision) and taking the recordings over time, /8, 11/.

POSSIBLE WORKFLOW AND FUTURE POSSIBILITIES

In the process of quantitative image analysis, there should be a well-designed workflow to ensure better and accurate end results. Artificial intelligence is set to revolutionise scientific research where complex data in large amounts can be visualised and interpreted by AI models. In parallel, the advancement and development of AI will enable a wide application of it in various fields (like medical, pharmaceutical, material science, etc.). In metallography, AI developments will make it possible to predict the lifetime of different metals, therefore raising awareness among engineers to overcome some problems which may likely happen such as building collapsing. In industrial field, AI development is likely to bring a positive effect through its increased efficiency, accuracy, and speed to handle much more complex patterns. The following cycles outline the industrial applications of future developed AI models, /8, 9/.

Cycle 1: the slurry preparation process, based on material AI, gives prediction about possible required data and information.

Cycle 2: casting parameter control process where AI can predict process parameters and transfer them to the device.

Cycle 3: quality validation processes and vision inspection system, AI visual inspection will make it possible to check the quality of products.

Cycle 4: process optimisation. AI will be able to learn, optimise itself and find best solutions for current material.

SOFTWARE DEVELOPMENT

The initial development of the software was focusing on cementite segmentation. A python-based software was made to summarise the results got by AI analysis and make predictions of future behaviour of the material in this actual condition. For the prediction we used the transfer learning and deep learning combination. Results of the initial execution of software appear promising and are converging with the results obtained from theoretical calculations, Figs. 3-6.

Applying several different theoretical approaches together gives a closer result to the real future behaviour of the crack. If the software database became wider with validated approaches, the final results will have better accuracy.

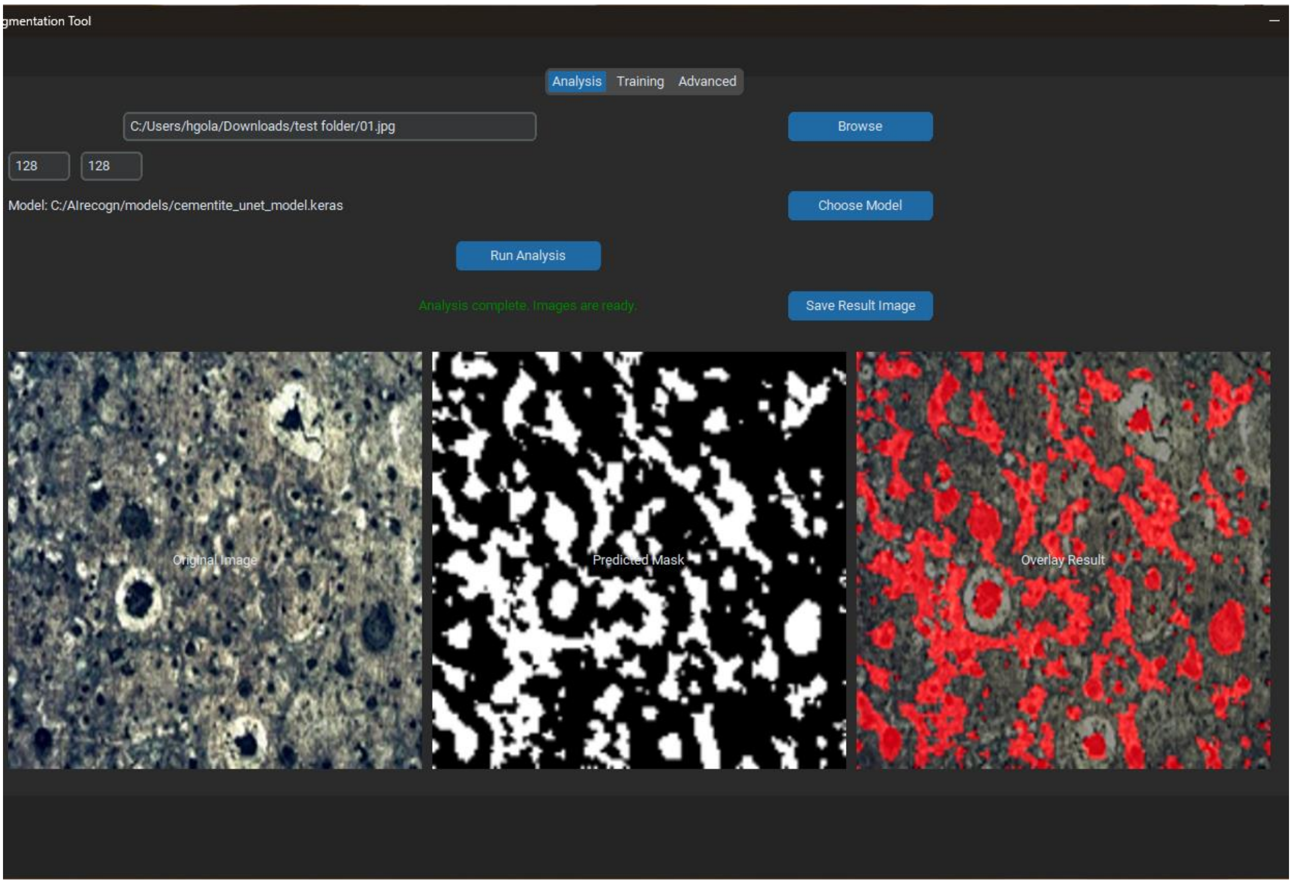

Figure 3. Cementite segmentation part of the software.

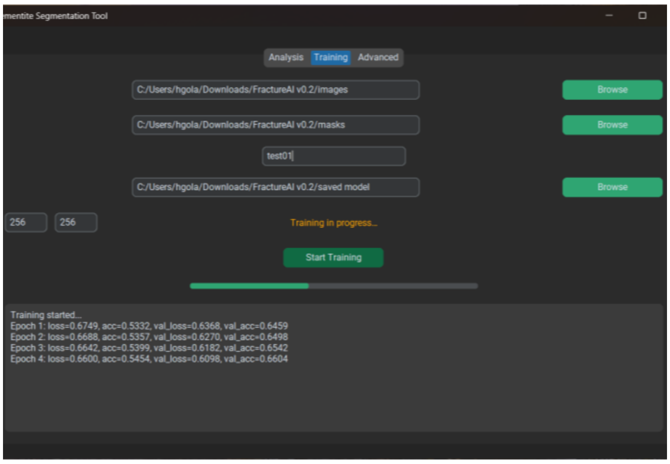

Figure 5. Training mode.

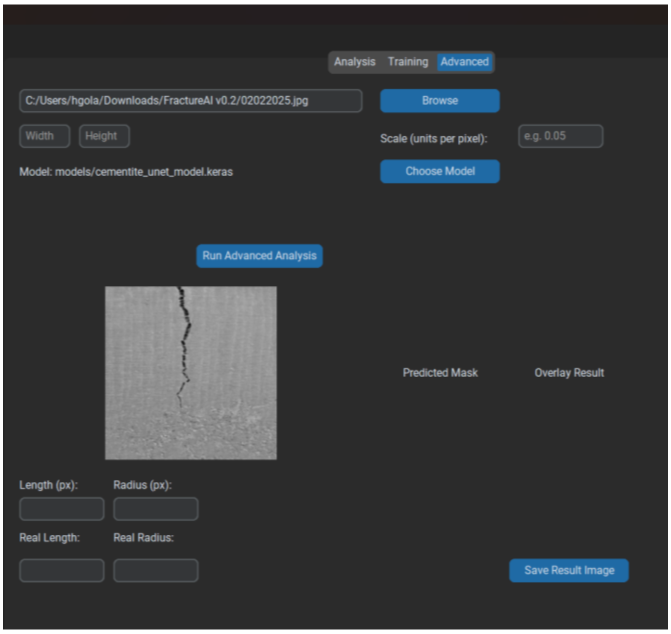

Figure 6. Crack sample detection and training of the module.

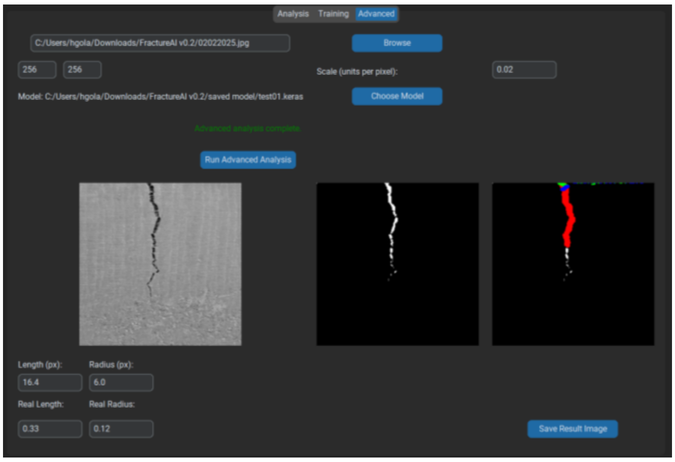

Figure 6. Crack propagation prediction by AI.

CONCLUSIONS

Artificial intelligence (AI) based methods for metallographic and quantitative image analysis play an important role in the analysis of materials. These methods help by laying down a clear view in understanding different properties of materials and defect detection in materials. In this article, we present the complexity of AI models parallel with highlighting different learning techniques employed to enhance AI models. In contrary, we outline the future applications of AI especially in material science. Furthermore, the development of AI gives a clear picture that in the future it can serve as an educational tool and more advanced computing microscope offering a wide range of microstructure variations at different enhancements. With various kind of AI based application development, based on new validated theoretical approach, this could be another possibility to increase the accuracy of structural integrity prediction by summarising all the known and available validated metallography and fracture mechanical theoretic knowledge base.

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