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AI Approach for Predicting Superhyrophobicity of Thermal Sprayed Copper Coated Aluminum Surfaces

Mahule Roy

Metallurgical and Materials Engineering Undergraduate, NITK Surathkal, India

ABSTRACT

Wettability, characterized by the contact angle of a liquid on a surface, is a critical property that influences numerous natural and industrial applications. In this study, I have developed a CNN-based model to predict the hydrophobicity or super-hydrophobicity of copper-coated aluminum surfaces treated with various reagents or etchants. The data set has been created by analyzing copper-coated aluminum samples with a 3D non-contact profilometer, and contact angle measurements were done to correlate surface properties with the resultant contact angle values. After reagent treatments, the approach had been to preprocess 3D profilometer images to extract surface morphology and structure features. These images and associated contact angle measurements were used as inputs to train the CNN model to classify whether the treated surfaces are hydrophobic or super-hydrophobic. Although the model may initially have limited training accuracy, this study demonstrates the potential of deep learning to predict wettability based on surface characteristics. The results also highlight the need for improvements, such as data set expansion, the inclusion of more varied reagent treatments, and the exploration of hybrid modeling approaches to enhance the model.

***Corresponding author**

Mahule Roy, Metallurgical and Materials Engineering Undergraduate, NITK Surathkal, India.

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Introduction

Wettability, the way a liquid interacts with a solid surface, is crucial in natural and industrial settings [1]. It dictates whether a liquid spreads across a surface or forms droplets, influencing applications like self-cleaning surfaces, anti-fogging coatings, water-repellent fabrics, biomedical implants, and microfluidic devices [2]. Wettability is measured by the contact angle, which forms at the point where the liquid, solid, and vapor meet. A smaller contact angle means better wettability (hydrophilicity), while a larger one suggests poor wettability (hydrophobicity). Surfaces with contact angles above 150° are super hydrophobic and show remarkable water-repelling properties.

Nature offers fascinating examples of diverse wettability traits shaped by evolution. For instance, the lotus leaf is a classic example of superhydrophobicity. Its surface, covered in microscopic and nanoscale structures, traps air and minimizes liquid-solid contact, allowing water droplets to roll off and clean the surface -a phenomenon called the "lotus effect." This natural design has inspired many innovations, like water-repellent and self-cleaning materials. In contrast. rose petals, while hydrophilic, show an interesting ability to hold water droplets firmly on their surface due to unique structural adaptations. These examples illustrate the intricate relationship between surface energy, roughness, and structure in determining wettability [3].

Traditionally, wettability is studied by measuring contact angles using methods like sessile-drop goniometry or the Wilhelmy plate technique. While effective, these approaches are time-intensive, require specialized equipment, and may not fully capture the complexities of surfaces with intricate structures, such as those in nature. This limitation is particularly evident in studying metals like copper and aluminum surfaces, where unique textures and patterns significantly influence wettability [4].

Artificial intelligence advances offer exciting new ways to analyze and predict wettability. Convolutional Neural Net- works (CNNs), a type of deep learning model specialized for image analysis, are particularly promising for identifying complex surface features. These models can detect hierarchical patterns in surface morphology, which are key to under- standing wettability. CNNs, therefore, hold great potential for exploring the relationship between surface features and wettability [5].

This research focuses on leveraging CNNs to predict the wettability of copper-coated aluminum samples using various etchants based on their morphological features. By analyzing high-resolution non-contact 3D-profilometer images of copper- coated aluminum surfaces, the study aimed to create a model that connects specific characteristics, like surface roughness, vein patterns, and textures, to measured contact angles.

Application of Superhydrophobicity in Biomedical Implants

In the biomedical domain, controlling surface wettability is crucial for applications like implant coatings, where superhydrophobicity can minimize bacterial adhesion and improve biocompatibility.

Copper-coated aluminum surfaces, when modified to exhibit controlled wettability, may of- fer new avenues in implant design. This study's methodology-leveraging CNNs to correlate surface morphology with wettability-can be extended to optimize implant surfaces by predicting and tailoring their wetting properties. Thus, the pro- posed AI-driven approach holds promise in developing next- generation biomedical implants with enhanced performance and reduced risk of infection.

Literature Review

Surface Wetting Characterization

Surface wettability is a crucial property influencing various natural and industrial processes, such as self-cleaning surfaces, anti-fog coatings, and biomedical applications. Wettability is often quantified by measuring the contact angle, which reflects the hydrophobicity or hydrophilicity of a material. Several analytical techniques have been developed to evaluate wettability, each offering specific strengths and limitations [1].

Existing Methods in Wettability Analysis

Sessile Drop Goniometry

Sessile-drop goniometry is one of the most commonly employed optical methods for measuring contact angles. The process involves placing a droplet of liquid on a solid surface and capturing the profile of the droplet using a high-resolution camera. The contact angle is determined through image analysis, typically utilizing Young's equation. Modern goniometers are often integrated with advanced image analysis software that provides detailed measurements of advancing and receding contact angles, thus offering valuable insights into the surface wettability and dynamic behavior.

Tilting Plate Method

The tilting plate method is a direct technique used to measure contact angles by analyzing a droplet's leading (advancing) and trailing (receding) edges as it begins to slide on an inclined surface. Adjusting the tilt angle of the plate allows for the evaluation of the droplet's mobility and its adhesion to the surface. The sliding angle, a key parameter in this method, indicates the droplet's mobility, making this technique particularly useful for studying dynamic wetting behaviors. This method is commonly applied in research involving surface lubrication and fluid dynamics.

Wilhelmy Plate Technique

The Wilhelmy plate method involves vertically immersing a thin solid plate into a liquid and measuring the forces exerted on the plate as it is submerged and withdrawn. The contact angle is calculated based on these force measurements, providing an accurate and reproducible method for determining wettability. This method benefits large sample areas and can be easily automated for high-throughput analysis. However, the Wilhelmy plate technique is less effective on rough or textured surfaces, as the challenges associated with defining the contact line can lead to measurement inaccuracies.

Axisymmetric Drop Shape Analysis (ADSA-P)

Axisymmetric Drop Shape Analysis (ADSA-P) is a technique that uses the shape of a droplet-either sessile or pendant-to calculate the contact angle and liquid-solid interfacial tension. The experimental profile of the droplet is compared to theoretical profiles derived from the Laplace equation. This technique is particularly advantageous for measuring contact angles on mineral surfaces or materials with relatively lowsurface roughness. ADSA-P provides accurate measurements of contact angles and surface tension, making it ideal for materials that exhibit minimal surface heterogeneity.

Microscopy Techniques

Microscopy methods, such as atomic force microscopy (AFM) and confocal microscopy, measure contact angles on small particles or irregular sur- faces. These techniques are beneficial for studying colloidal particles in aqueous solutions and measuring forces between a bubble and a colloidal particle. Although these methods provide highly detailed data on surface interactions, they re- quire complex experimental setups and extensive data analysis, which limits their use for routine contact angle measurements. Despite these challenges, they offer significant advantages for nanoscale investigations and specialized applications.

Study of Etchants used for Making Cu Surface Hydrophobic

As part of the literature review, I compiled a list of papers detailing the etchants that can render copper surfaces hydrophobic or super hydrophobic. These etchants are crucial for the study as I have applied the etchants to modify the surfaces and then conducted our analysis using various techniques [5-7].

Emerging Approaches in Wettability Analysis

While conventional methods for wettability analysis remain crucial for understanding surface behavior, their limitations, such as the need for large sample areas, susceptibility to human error, and complexity, have led to the exploration of advanced techniques, including artificial intelligence. In particular, deep learning models, notably Convolutional Neural Networks, have shown great promise in automating the analysis of surface textures.

Objective of the Study

The primary objective of this research was to develop a deep learning-based model designed to predict the wettability of copper-coated aluminum surfaces. This was accomplished through the use of convolutional neural networks (CNNs), which are well suited for analyzing visual data due to their powerful capabilities in feature extraction and pattern recognition. The model was trained to process images of coated surfaces and automatically identify visual patterns and characteristics that are indicative of different levels of wettability. By learning from a diverse set of image data, CNN was able to make accurate predictions without the need for manual interpretation or traditional measurement methods.

This approach was intended to provide a faster, more efficient and more objective alternative to conventional analysis techniques. Reduce human error and accelerate the evaluation process, making it particularly useful in industrial and research settings where time and accuracy are critical. The study aimed to validate the use of CNNs in materials science applications, showcasing their ability to assess surface properties from visual input alone.

Through this work, the potential of deep learning techniques in surface characterization was highlighted, demonstrating their broader applicability in surface engineering and predictive modeling. By bridging machine learning with materials science, research contributes to the development of intelligent systems capable of supporting material design, quality control, and performance analysis. Ultimately, the study established a robust, data-driven framework for predicting surface wettability, paving the way for more advanced and automated analysis tools in the field.

Methodology

Data Collection

I created a dataset on various copper-coated aluminum samples obtained for my use. First, I took a sample, and then I precisely cut it into the shape of squares and rectangles. Then, the samples were etched using various combinations of etchants [6]. The etchants I used, after referring to different papers, are

- FECl
- Hydrochloric acid
- 0.005 mol/L ethanol solution of stearic acid for 5 min

Figure 1: Etchants used for Etching the Copper Coated Aluminum Surface

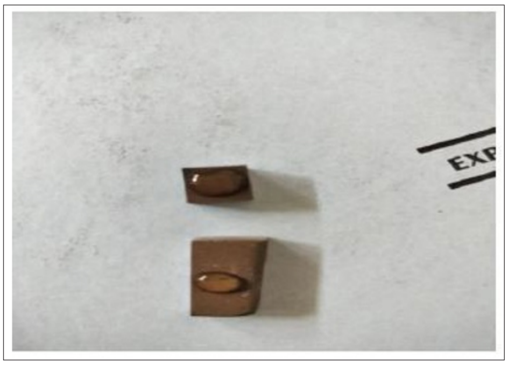

Figure 2: Copper Coated Aluminum Samples

Wettability Measurements

Contact angle values measured through conducting experimental setups. The methodology used to determine the contact angle:

1. Surface Preparation and Droplet Deposition: The surface had to be smooth to ensure accurate measurements. A precise volume of liquid (typically water or another appropriate liquid) was dispensed onto the surface using a droplet dispenser. The size of the droplet was controlled to ensure consistent and accurate measurements. The droplet was placed gently on the surface to avoid splashing or disturbing the surface.
2. Imaging the Droplet: Once the droplet was placed on the surface, a high-resolution camera captured the profile of the droplet. The camera was positioned directly above the droplet to obtain a clear image of the droplet resting on the surface.
3. Image Analysis Using Software: The software captured the image of the droplet in real-time or from a series of frames. A single image is typically sufficient for static contact angle measurement. The software detects the edges of the droplet, identifying the liquid-solid interface. The droplet's shape was then fitted to a theoretical model. (often a circular or polynomial curve), allowing the software to analyze the shape and determine the contact angle.
4. Contact Angle Calculation: After fitting the droplet profile, the software calculates the contact angle. The contact angle was formed between the tangent to the droplet at the contact point and the material's surface. The software outputs the contact angle directly, providing a numerical value that reflects the surface's wettability.

- A contact angle less than 90° indicates a hydrophilic surface, where the liquid spreads across the surface.
- A contact angle greater than 90° indicates a hydrophobic surface, where the liquid beads up and resists spreading.
- A contact angle greater than 150° indicates a super hydrophobic surface, where the liquid beads up and resists spreading.

3D Profilometer Images of Etched Copper Surfaces

I have captured 3D profilometer images of the etched surfaces to provide a more comprehensive analysis. The model were fed these images to enhance its understanding of surface properties and their correlation with surface morphologies.

Feature Extraction

Morphological features are quantified using image processing and microscopy techniques, focusing on:

- Surface roughness and micro-textural patterns.
- Surface geometry, which is crucial for predicting how water interacts with the etched surface.

Prediction Model Used: Convolutional Neural Network

In this study, a convolutional neural network (CNN) was employed to predict the wettability of copper surfaces by analyzing their morphological characteristics. CNNs are particularly well-suited for handling image data due to them.

Figure 3: Kruss Drop Angle Analyzer

Ability to automatically extract and learn spatial hierarchies of features from visual inputs. By examining images of the copper surface, the CNN can identify intricate patterns, textures, and structural details that influence wettability. This capability makes CNNs a powerful tool for understanding and modeling the relationship between surface morphology and wettability. Unlike traditional image analysis methods that rely on manual feature extraction, CNNs learn relevant features directly from the data, enabling more accurate and efficient predictions [7].

Procedure

Below is the procedure followed for implementing the code based on the dataset compiled after contact angle measurements and 3D Profilometer:

- After receiving 300 images (12 samples) from the 3D Profilometer I first separated the images into two folders, one of hydrophobic and another of superhydrophobic.
- After the images were separated into two classes, I then implemented the code which will extract the red regions

from the obtained images, this was done since I wanted to relate the red regions with higher surface roughness value.

- The bounding box implementation is a method to make the model understand that it had to prioritize the red regions and based on that red region area to total area calculation, it would predict the provided image as being hydrophobic or super hydrophobic.
- Next, to make the prediction accuracy stronger we implemented a Convolutional Neural Network (CNN) to read in the images with the bounding box to relate it with the surface roughness based on the red region area calculation. CNNs are extremely good at handling images and because of our case I found it to suit our requirement the best.

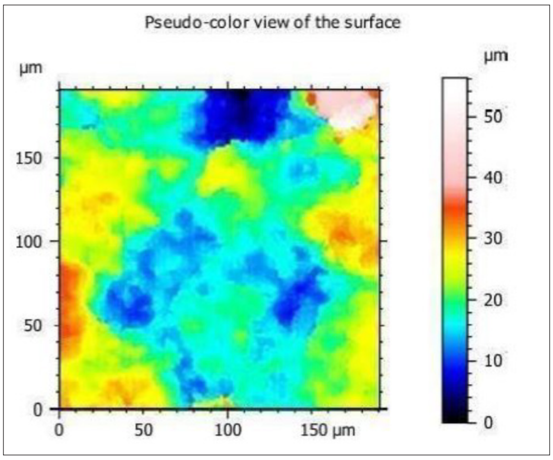

Figure 4: 2D View of an Image Taken by a 3D Noncontact Profilometer

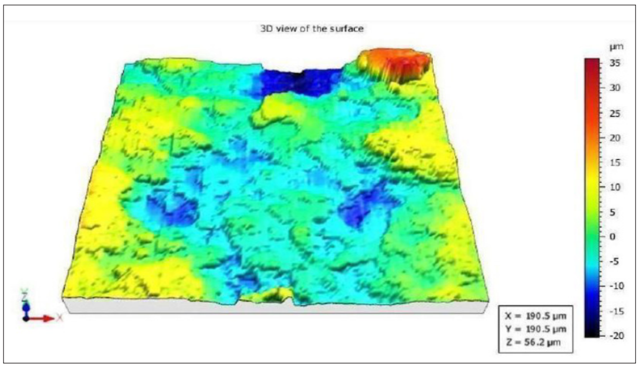

Figure 5: 3D View of an Image Taken by a 3D Noncontact Profilometer

```python
from tensorflow.keras.layers import Input, Dense, Conv2D, MaxPooling2D, Flatten, Concatenate, Dropout
from tensorflow.keras.models import Model

def build_hybrid_model(image_shape):
    image_input = Input(shape=image_shape, name="image_input")
    x = Conv2D(32, (3,3), activation='relu')(image_input)
    x = MaxPooling2D()(x)
    x = Conv2D(64, (3,3), activation='relu')(x)
    x = MaxPooling2D()(x)
    x = Flatten()(x)
    red_area_input = Input(shape=(1,), name="red_area_input")
    y = Dense(16, activation='relu')(red_area_input)
    combined = Concatenate()([x, y])
    z = Dense(64, activation='relu')(combined)
    z = Dropout(0.5)(z)
    output = Dense(2, activation='softmax')(z)
    model = Model(inputs=[image_input, red_area_input], outputs=output)
    model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])
    return model
```

Figure 6: Convolutional Neural Network Architecture Used

- The next step was to get these predictions from the CNN and then link it up with our handmade CSV file containing the information for each 12 samples regarding the etchants used for them, time of etching, contact angle measured, and ratio of the etchants used.
- This CSV helped in making the model understand the relation between surface roughness, contact angle, use of etchants etc. Due to this the model was able to recommend based on the input of a 2D view of an image taken by the 3D Profilometer.
- This recommendation contained the following parameters – ratio of etchants, etchants that can be used, time of etching, possible angle of contact, and also prediction on the surface being hydrophobic or superhydrophobic.
- These were the steps I followed to implement the deep learning code. This code was further optimized using various other methods and techniques to make the pre- diction faster which was my main objective since the conventional methods lack this.

Optimization

My main objective of going for deep learning was to make the entire process of prediction faster than the traditional method, so to ensure this I had implemented various optimization methods as part of the code.

- Dropout - is a regularization technique where, during training, a random subset of neurons in a layer is temporarily deactivated (i.e., their output is set to zero). Each neuron normally receives inputs, applies weights and an activation function, and passes the result forward. By randomly turning off neurons, dropout prevents the network from becoming overly reliant on specific neurons, forcing it to distribute learning across many. This leads to more robust internal representations and helps reduce overfitting. During testing, all neurons are active, but their outputs are scaled to account for the dropout applied during training.
- Reduce LR On Plateau - This tool slows down learning when your model stops getting better. If the model's performance (like validation loss) doesn't improve for a few rounds (epochs), it lowers the learning rate so the model can make finer adjustments.
- Early Stopping - This stops training if the model hasn't improved after a few tries. It helps save time and prevents the model from overfitting (memorizing the training data too much).
- Data Augmentation - is a technique used to improve a machine learning model's performance by creating modified versions of the existing training data. In image tasks, this often involves transformations like flipping, rotating, zooming, cropping, or adjusting brightness. These changes help the model learn to recognize patterns under different conditions, making it more general and less likely to overfit. Even though the data is artificially changed, the meaning or label stays the same, which helps the model learn what features truly matter.
- Using the above techniques, I was able to make the code run and execute much faster in comparison to the conventional methods which was my main objective when starting out.

Results

To validate the model performance, I used various metrics like training accuracy and validation accuracy to understand the model's performance. A little bit more on the metrics I used:-

- Training accuracy is the percentage of correct predictions the model makes on the data it was trained with. It shows how well the model is learning that specific dataset.

- Validation accuracy, on the other hand, is the percentage of correct predictions on a separate set of data the model hasn't seen before, used to check how well it can generalize to new inputs.
- If training accuracy is high but validation accuracy is low, it often means the model is overfitting — it memorizes the training data but doesn't perform well on new data.

These below results were achieved over 11 epochs (training steps) and attached is the output screenshot for the perfor- mance seen over 11 epochs showing the training and validation accuracy values over each run the model performs.

- Training Accuracy = 65
- Validation Accuracy = 60

```
Epoch 1/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 10s 1s/step - accuracy: 0.5176 - loss: 576.0433 - val_accuracy: 0.5500 - val_loss: 17.1098 - learning_rate: 0.0010
Epoch 2/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 6s 725ms/step - accuracy: 0.5800 - loss: 17.4026 - val_accuracy: 0.5500 - val_loss: 2.0740 - learning_rate: 0.0010
Epoch 3/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 12s 879ms/step - accuracy: 0.5455 - loss: 1.4151 - val_accuracy: 0.5500 - val_loss: 3.7349 - learning_rate: 0.0010
Epoch 4/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 9s 841ms/step - accuracy: 0.5500 - loss: 3.5318 - val_accuracy: 0.5500 - val_loss: 0.7146 - learning_rate: 0.0010
Epoch 5/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 9s 692ms/step - accuracy: 0.6355 - loss: 0.6954 - val_accuracy: 0.5500 - val_loss: 0.7142 - learning_rate: 0.0010
Epoch 6/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 8s 991ms/step - accuracy: 0.6186 - loss: 0.6923 - val_accuracy: 0.5500 - val_loss: 0.7029 - learning_rate: 0.0010
Epoch 7/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 8s 702ms/step - accuracy: 0.6424 - loss: 0.6714 - val_accuracy: 0.5667 - val_loss: 0.6927 - learning_rate: 0.0010
Epoch 8/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 11s 816ms/step - accuracy: 0.5638 - loss: 0.6717 - val_accuracy: 0.5167 - val_loss: 0.6924 - learning_rate: 0.0010
Epoch 9/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 10s 726ms/step - accuracy: 0.6819 - loss: 0.6471 - val_accuracy: 0.6000 - val_loss: 0.6937 - learning_rate: 0.0010
Epoch 10/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 7s 927ms/step - accuracy: 0.6435 - loss: 0.6119 - val_accuracy: 0.5667 - val_loss: 0.7232 - learning_rate: 0.0010
Epoch 11/30
8/8 ━━━━━━━━━━━━━━━━━━━━ 9s 728ms/step - accuracy: 0.6379 - loss: 0.5878 - val_accuracy: 0.5500 - val_loss: 0.7290 - learning_rate: 5.0000e-04
Epoch 1: Train Accuracy = 0.4917, Validation Accuracy = 0.5500
Epoch 2: Train Accuracy = 0.5708, Validation Accuracy = 0.5500
Epoch 3: Train Accuracy = 0.5542, Validation Accuracy = 0.5500
Epoch 4: Train Accuracy = 0.5500, Validation Accuracy = 0.5500
Epoch 5: Train Accuracy = 0.6000, Validation Accuracy = 0.5500
Epoch 6: Train Accuracy = 0.6042, Validation Accuracy = 0.5500
Epoch 7: Train Accuracy = 0.6500, Validation Accuracy = 0.5667
Epoch 8: Train Accuracy = 0.5625, Validation Accuracy = 0.5167
Epoch 9: Train Accuracy = 0.6750, Validation Accuracy = 0.6000
Epoch 10: Train Accuracy = 0.6625, Validation Accuracy = 0.5667
Epoch 11: Train Accuracy = 0.6417, Validation Accuracy = 0.5500
```

Figure 7: Output Screenshot of Model Performance (Training and Validation Accuracy)

Based on the 3D Profilometer image provided by the user, I have made a recommendation deep learning model which can possibly comment on the nature of the surface i.e. Hydrophobic or Superhydrophobic, etchants ratios that can be used, the time for etching, and the angle of contact. This recommendation code was implemented based on the CSV which contains the information regarding the experiments performed by me as part of the dataset creation process. The output screenshot below shows the abilty of the model to suggest such parameter values based on the 2D view image provided by the user. This ensures that the implemented model can be used by other researchers to get accurate predictions.

```
1/1 ━━━━━━━━━━━━━━━━━━━━ 0s 50ms/step
Predicted Class: Hydrophobic
Recommended Contact Angle: 138.0°
Recommended Etchants: FeCl3=0.0, Hcl=1.0, Stearic Acid=1.0
Recommended Time: 40.0 seconds
<ipython-input-78-53c85b95b4cd>:6: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead
```

Figure 8: Recommendation Code of the Model

The model can also draw bounding box to specify the red regions which are crucial for predicting the contact angle and surface roughness. The red regions correspond to higher surface roughness and more red regions implies that the 2D view image of the sample is superhydrophobic. Below is the output screenshot where the model has drawn bounding boxes to highlight the red regions.

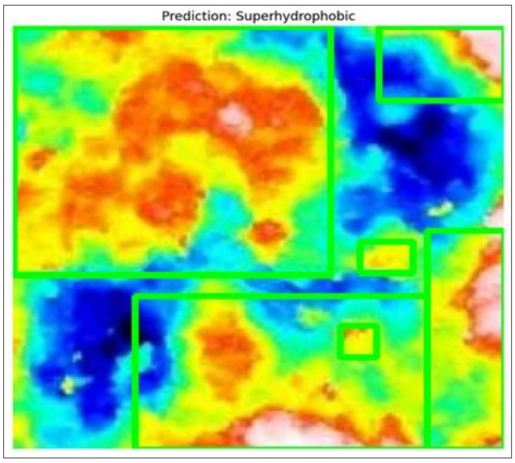

Figure 9: Bounding Box of Super Hydrophic 2d View Image Around Red and Yellow Regions for Higher Surface Roughness Detection

Conclusion

- Investigated the use of chemical etchants to engineer superhydrophobic copper-coated aluminum surfaces and evaluate their wettability using deep learning, specifically convolutional neural networks (CNNs).
- To understand how chemical modifications of copper's surface morphology affect its wetting behavior. This was done by modifying micro and nanoscale features of copper surfaces using different chemical etchants and their ratios.
- Captured high-resolution images of the chemically treated surfaces and used CNNs to analyze these images. CNNs are highly effective at recognizing complex patterns and extracting features from images, it can detect morphological differences that traditional image analysis may miss.
- Explored the correlation between surface topography and wettability. I aimed to develop a predictive model to estimate contact angles or superhydrophobicity levels based on images.
- Demonstrated the potential of machine learning in materials science. I was able to develop an efficient and automated method for predicting and designing surface properties. These findings can benefit fields like coatings, sensors, and microfluidics.
- This was my first attempt at trying to figure out how to use AI to predict super hyrdophobic surfaces, though this is an attempt at exploring the field in detail, I want to extend my idea further to SEM images.

Future Scope

The application of deep learning techniques, particularly convolutional neural networks (CNNs), in predicting the wettability of copper-coated aluminum surfaces opens several promising avenues for future research and technological advancement.

- Integration with Advanced Imaging Techniques: Future work can explore combining deep learning models with high-resolution imaging tools such as scanning electron microscopy (SEM) or atomic force microscopy (AFM) to gain deeper insights into surface morphology and enhance prediction accuracy.
- Real-Time Wettability Prediction: Developing lightweight, optimized CNN models suitable for deployment on edge devices could allow for real-time, on-site wettability assessment in industrial environments.
- Scalability to Other Materials: The approach demonstrated for copper-coated aluminum surfaces can be ex- tended to

study wettability in a wide range of materials like aluminum, which is mainly used in the aerospace industry, to make it more corrosion resistant.

- Standardization and Dataset Expansion: Creating large, standardized datasets of surface images and wettability measurements will support broader adoption of deep learning methods and enable more accurate benchmarking across models.

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