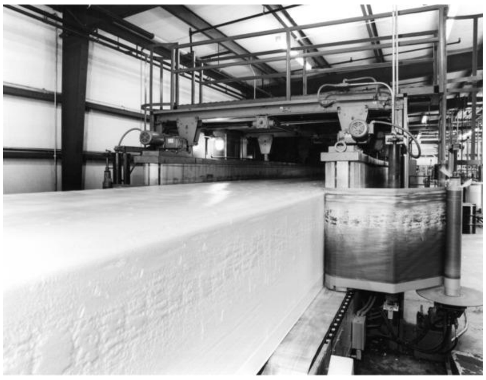
Computer Vision

Final project: Exploring the Microstructure of Polyurethane Foams: A Machine Learning Approach

1. Introduction

Polyurethanes are a class of polymers that span a vast spectrum of applications, thanks to their unique attributes like flexibility, resilience, and the ability to form materials with varied densities and hardness levels. They permeate a multitude of industries, from automotive to furniture, packaging to construction, and truly stand as one of the most versatile synthetic materials available in the market.
Polyurethane foams, a distinctive subclass of polyurethanes, are porous, lightweight materials. Their unique attributes stem from the foaming process, which gives rise to small gas bubbles trapped within the material matrix. The adjustability of polyurethane foams, in terms of their cellular structure, density, and hardness, makes them remarkably adaptable materials.



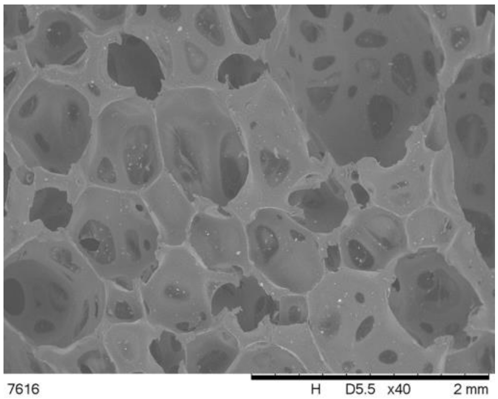


Fig. 1-2. Flexible polyurethane foam manufacturing line (left); SEM image of microstructure (right)

In Poland, the polyurethane foam sector holds significant economic prominence. The country stands as one of the largest manufacturers and exporters of polyurethane foams in Europe (TOP1 largest manufacturer of upholstered furniture), a fact that translates to substantial employment opportunities and a notable contribution to the country's Gross Domestic Product (GDP). Moreover, this sector is continually evolving and innovative, placing Poland at a key position on the global map of the polyurethane industry. There is a huge business need to product high quality functional polyurethane materials.

In R&D process when you're working on new tailor-made material formulation the most important factors are time and money. Materials have different mechanical, physical, thermal, etc. properties. For manufacturers in automotive, physiotherapy and mattresses industries one of the most important are mechanical properties, because they determine the comfort of the user and the durability of the product. The key factor that indicates the material is microstructure. It is commonly known that there is huge relation between the structure and properties. The comprehension of the structure and properties of polyurethane foams is crucial for their ongoing development and optimization. Therefore, the analysis of images from Scanning Electron Microscopy (SEM), which allows the visualization of the cellular structure (is a powerful tool in the realm of material science, allowing for the visualization of material structures at the microscopic level), is pivotal in the context of research and innovation related to these materials.

The microstructure of flexible polyurethane foams can reveal a wealth of information about their physical and mechanical properties. This analysis primarily involves examining the size, shape, and distribution of the cells (tiny gas-filled bubbles) within the foam. From the microstructure of the foams we can read and interpret:

- cell size - the size of the cells can influence the density and mechanical properties of the foam. Smaller cells usually result in denser and stronger foams, while larger cells lead to lighter and softer foams. Moreover, cell size can also affect the thermal and acoustic insulation properties of the foam.

- cell shape - the shape of the cells (whether they are more spherical or elongated) can provide clues about the manufacturing process and conditions. It can also influence the material's properties; for instance, more elongated cells can contribute to anisotropic behavior in the foam, meaning the properties vary depending on the direction of measurement.
- cell distribution - a uniform cell size distribution usually leads to more predictable and consistent material properties. In contrast, a wide distribution can lead to variability in properties throughout the material.
- cell wall thickness: the thickness of the cell walls, or "struts," can affect the strength and rigidity of the foam. Thicker walls usually result in stronger foams.
- open vs. closed cells - the ratio of open to closed cells can significantly influence the material's properties. Open-cell foams allow gas and liquid to pass through and are typically softer and less rigid than closed-cell foams. They are used in applications like cushioning and padding. Closed-cell foams, with their gas-tight cells, provide excellent insulation and buoyancy and are used in applications like insulation panels and flotation devices.

Through SEM imaging and microstructure analysis, we can optimize the production process and tailor flexible polyurethane foams to specific applications, meeting precise property requirements.

It's important to note that these microstructural characteristics are interconnected, meaning a change in one can influence others, and ultimately, the foam's properties. As it was said before, crucial in R&D process is to minimize costs and save time to prepare new formulation. It was hypothesized that Computer Vision might be helpful to reduce some of the tests – learn some features of images to predict mechanical properties (in this case a tensile force that stretches the material to 40% of its original length).

2. Tools and technologies

For the successful completion of this project Python, PyTorch and Google Colab were used. The choice of tools was guided by their ease of use, community support, and suitability for the task at hand. PyTorch as a machine learning library offers a rich API for neural network layers, loss functions, optimization alghoritms and tools for loading and preprocessing data. Google Colab is a free cloud service that offers access to computing resources, including GPU's, which are particularly useful for training complex neural network models.

3. Dataset

The dataset utilized for this project consists primarily of Scanning Electron Microscope (SEM) images of polyurethane foams, taken at magnifications of 40, 50, 100, 250, and 1000 times. However, the bulk of the images were obtained at a magnification of 40x, which served as the core of the dataset.

In the initial stages of the project, experiments were conducted using images from all levels of magnification. However, in the final iteration of the project, the focus was narrowed to include only the 40x magnified images. This decision was made based on the consistency of the results and the computational efficiency provided by these images.

The dataset reflects the diversity of the foam's microstructure, with each image representing a unique aspect of the material's properties. The dataset covers 19 different polyurethane foams, each synthesized with a different chemical composition. For each type of foam, approximately 35-50 images were captured at various locations across the material's cross-section, providing a comprehensive visualization of the foam's structure.

Alongside the SEM images, a dataset containing the mechanical properties of the foams was also available, including the critical property of 40% tension. This mechanical property is an essential characteristic that describes the foam's stress-strain behavior under specific conditions of strain.

The original dimensions of the images were 1280x1040 pixels, ensuring a high level of detail. However, to accommodate computational constraints and maintain a consistent input size, the images were resized for the machine learning model.

4. Experiments

4.1. Dataset creation

The first step involved generating a custom dataset based on the provided raw input. The Python ‘os’ library facilitated the organization and collation of image paths and corresponding properties, effectively creating a comprehensive record of our data sources.

4.2. Data visualization

In order to understand the dataset more intuitively, custom visualization functions were developed. These not only displayed random images along with their associated properties and sample labels but also provided insights into the transformations performed on the images.

4.3. Data transformation

The subsequent phase involved transforming images into tensors, a format compatible with our neural network models. We utilized the transforms.Compose functionality provided by the PyTorch library for this purpose. These tensors were then normalized according to the mean and standard deviation inherent to the Resnet architecture, to maintain consistency and facilitate efficient training.

4.4. Data batching and iteration

To handle the computational load efficiently and enable the optimization algorithm to work effectively, the data were organized into batches. By making these batches iterable, the feeding process was streamlined into models during the training and testing stages.

4.5. Training and testing loop

At the core of the experimentation phase was the design and implementation of training and testing loops for our neural network models. To prevent overfitting and achieve robustness in our models, an 'early stopping' mechanism was introduced. If no decrease in the test loss was observed for three consecutive iterations, the training process was interrupted, saving computational resources and time.

4.6. Transfer learning application

Harnessing the power of transfer learning, we tested pretrained models on our dataset. These models were adapted to our regression problem and their weights were employed as a starting point, offering the advantage of proven, reliable feature extraction abilities. Among the architectures explored were Resnet50, Resnet34, and EfficientNet.
This methodical approach enabled the development of robust models capable of predicting properties from SEM images, advancing the capabilities in the field of polyurethane foam material analysis.

4.7. Custom model

In addition to the established models adapted through transfer learning, a novel architecture inspired by TinyVGG was also designed and tested. Named as SEMNet, this custom architecture was tailored specifically for the dataset and the regression task at hand.
The SEMNet architecture consists of two main sections: the convolutional blocks and the classifier.
The first part of SEMNet is comprised of two convolutional blocks, each following a specific pattern: Convolutional layer -> Activation function (ReLU) -> Convolutional layer -> Activation function (ReLU) ->

Max Pooling layer. The purpose of these blocks is to extract the relevant features from the input SEM images.

Each Convolutional layer in the block has a kernel size of 3, with the first layer having a stride of 1 and padding of 1, while the second layer has no padding. After each Convolutional layer, the Rectified Linear Unit (ReLU) activation function is applied, introducing non-linearity into the model.

Following these layers, a Max Pooling layer is applied with a kernel size of 2 and a stride of 2, to reduce the spatial dimension of the output from the previous layers, and to assist in capturing the most salient features.

The second part of SEMNet is a classifier, which consists of a Flatten layer, followed by a fully connected Linear layer. The Flatten layer transforms the 2D output of the previous convolutional block into a 1D tensor, which then serves as the input to the Linear layer.

The Linear layer maps these inputs to the final output shape, producing the desired property prediction from the input SEM image. This output is directly returned by the forward function of SEMNet, providing the model's prediction for the input.

4.8. Various experimentation and analysis

Throughout the study, numerous trials were conducted to understand the performance of various configurations and approaches, as well as to optimise the predictive model for the given dataset.

4.8.1. Property predictions

The initial phase of experimentation involved predicting not only the 40% tension property but also other thermal and SAG factor properties. While these properties showed correlations with the SEM image structures to various extents, the mechanical property predictions (specifically the 40% tension) consistently provided the best results. This observation aligns with domain knowledge indicating that mechanical properties have a strong dependency on the material's microstructure.

4.8.2. Data transformations and augmentation

The study also explored the impact of different image transformations on the performance of the model. These transformations included image resizing to various dimensions. Furthermore, data augmentation techniques, such as image rotation, were introduced into the pipeline. Interestingly, the inclusion of data augmentation resulted in improved performance, suggesting that these techniques were successful in enriching the dataset and reducing the risk of overfitting.

4.8.3. Hyperparameter tuning

Another crucial aspect of the study was hyperparameter tuning. This involved testing various batch sizes ranging from 1 to 64, and diverse learning rates from 0.00001 to 0.1. Additionally, several loss functions, including Mean Squared Error (MSE), L1Loss, and SmoothL1Loss from the torch.nn library, were investigated. The MSE loss function proved to be the most effective for this task.

Various optimisers, including Stochastic Gradient Descent (SGD), Adam, and RMSprop, were also trialled. Adam was found to deliver the best results in terms of model performance.

For the custom SEMNet architecture, various sizes of hidden layers in the convolutional networks were examined. This process allowed for further fine-tuning of the architecture to optimally suit the specific characteristics of the SEM images.

4.9. Model evaluation

The assessment of the model's performance was a critical component of this study. Two primary strategies were adopted for this purpose: learning curves analysis and visual comparison of actual vs. predicted values.

Learning curves, which graphically represent the change in learning loss over training epochs, served as an indispensable tool in this study. They were used to monitor the model's learning process and to ensure that it was neither overfitting nor underfitting. The overfitting phenomenon, wherein a model performs well on the training data but poorly on unseen data, would have manifested as a significant divergence between the training and validation loss over time. Conversely, underfitting, where the model fails to capture the underlying patterns in the data, would have been indicated by persistently high training and validation losses.

By closely examining the learning curves, it was possible to gauge the model's performance and make necessary adjustments to the learning process. For instance, the early stopping technique was implemented to halt training when the validation loss ceased to decrease after a certain number of epochs, thus preventing overfitting.

In addition to the analysis of learning curves, the predicted values were plotted against the actual values for visual comparison. This allowed for an intuitive assessment of the model's performance and the opportunity to identify any systematic deviations or anomalies in the predictions. By visually comparing the predicted and actual values, it was possible to gain a deeper understanding of the model's strengths and limitations, as well as to determine the next steps for model refinement.

5. Results

Throughout the course of this study, multiple models were evaluated and compared, with a primary focus on our custom model and the ResNet50 architecture. The results showed a promising potential for Computer Vision applications in analyzing the microstructure of flexible polyurethane foams, particularly in predicting the 40% tension property.

Custom SEMNet model emerged as the superior model, performing slightly better than the ResNet50. This model effectively confirmed the relationship between the microstructure and 40% tension, a critical property of the polyurethane foams. On the other hand, the models' performance on predicting other properties was not as impressive, delivering results close to random prediction. This could suggest that these other relationships may not be as straightforward or may not be as directly related to the microstructure as the 40% tension property.

Hyperparameter optimization proved to be a challenging task, involving extensive testing and refinement of various values. The findings highlighted the need for a low learning rate, at least 0.0001, to achieve the best results. The Adam optimizer and Mean Squared Error (MSE) loss function were identified as the most effective components for our model's configuration.

Nevertheless, the models are not without their limitations. Factors such as a limited dataset, a lack of diversity in the properties, or the inherent complexity of the phenomena being studied could have contributed to the imperfections in the models. This emphasizes the importance of further investigation and model refinement to improve the performance and reliability of the predictive models in such complex tasks.

6. Sources

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