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Computer Vision and Machine Learning Making The Processing-Microstructure-Property Connection In Heat Resistant Alloys

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Processing-microStructure-Property connection



PSP connection: A fundamental tenet of materials science is that Processing generates the microStructure that mediates material Properties

Microstructure: the key link between what we control (processing parameters) and what we achieve (material property)

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machine learning for exploring PSP connection



Given its ability to find relationships in large, complex data sets, machine learning (ML) seems tailor-made for exploring PSP connections.

In this project, we develop and apply computer vision (CV) tools to create quantitative representations of microstructural images and apply ML methods to answer the question: *Can we predict material properties from images of the material microstructure?*

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pipeline

- 1. Collect microstructural image data and property metadata for heat resistant alloy systems.
- 2. Develop CV techniques to extract knowledge from microstructural images.
- 3. Create ML systems to find relationships between microstructures and property metadata.
- 4. Analyze and interpret the results to discover new PSP connections.

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Datasets – image data and property metadata



HR-53

n UTS (MPa) stdv (MPa) YS 0.2 (MPa) stdv (MPa) AR stdv EL stdv note Alloy T (C) HR52-T1 25 691.8 599.1 1.7 23.5 0.8 processed at 740 C 1.7 HR53-T1 25 722.8 1.1 590.6 0.8 21.75 0.1 processed at 740 C 739.8 16.9 594.8 127 22.7 HR54-T1 25 0.4 processed at 740 C HR58-T1 742.3 591.34 23.2 Poor surface finish, galled threads, tapered gage. HR62-T1 25 603.6 425.28 64.9 33.97 newly machined tensile sample. Tested on 4/27/2021. processed at 740 C HR63-T1 25 608.4 419.58 61.5 34.29 newly machined tensile sample. Tested on 4/27/2021. processed at 740 C HR66-T1 25 620.4 445.39 64.7 33.45 newly machined tensile sample. Tested on 4/27/2021. processed at 740 C HR67-T1 25 643.1 472.97 50.4 30.43 newly machined tensile sample. Tested on 4/27/2021. processed at 740 C HR68-T1 25 680.2 511.73 58 28.92 newly machined tensile sample. Tested on 4/27/2021. processed at 740 C HR71-T1 25 957.3 864.97 57.6 17.86 newly machined tensile sample. Tested on 4/27/2021. processed at 1015 C

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HR-66

Computer vision and CNN





Computer vision: is a field of artificial intelligence (AI) that **enables computers and systems to derive meaningful information** from digital images, videos and other visual inputs

Most computer vision algorithms use **convolution neural networks**, or CNNs. A CNN is a model used in machine learning to extract features, like texture and edges, from spatial data

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CNN - VGG16



Prediction of yield stress on 3 sample series





HR-53: 590.6 MPa HR-66: 445.39 MPa HR-68: 511.73 MPa **Carnegie Mellon University**

Feature visualization



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Yield stress prediction by regression model



Prediction error is the difference between true value and predicted value. In our research, we define the accurate prediction as the prediction within +- 15 MPa considering that experimental error of measuring yield stress. The prediction accuracy is **87.2%**.

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Prediction of yield stress on 7 sample series





Can we predict the YS for the different classes with very close YS just based on their visual difference?



Feature visualization



Key issue:

- recognize the difference between inter-class (largely different YS) and intra-class (close YS)
- 2. distinguish the similarity of intra-class (close YS)



Accurate yield stress prediction





accuracy within 15 MPa prediction error: 96.35%



Comparison of regression models



accuracy within 15 MPa prediction error: much narrower distribution with improved regression process 14

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Summary

In order to answer the question:

Can we predict material properties from images of the material microstructure?

- 1. Image data and property metadata are built to explore PSP connection
- 2. Data is selected and processed for CV/ML tasks
- 3. VGG16 is used to extracted features from image dataset and the characteristic features are used to make connection between the property
- 4. VGG16 shows high interpretability via feature representation method t-sne
- 5. Regression models are well built to predict yield stress (property) of heat resistant alloy (microstructure). The prediction accuracy can be as high as 96.35%



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Thank you !

