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CASE STUDY

Understanding and improving steel performance at OCAS

Executive summary

Leading steel research centre, **OCAS** (a joint venture between **ArcelorMittal** and the Flemish regional government) has used Alchemite™ deep learning to model the behaviour of steels. Key objectives for the project included: determining whether the method was effective for real-world, sparse data; finding out whether image data from microstructural analysis could add value to the machine learning models; and gaining insight into Processing - Structure - Property ('PSP') relationships. Alchemite™ was able to build models with high accuracy, improving its predictive power by extracting hidden information from microstructural images. Outputs from the project could be applied to focus valuable experimental resources more efficiently and to find new processing parameter combinations that meet specific target property requirements for steels.

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The challenge

> **Improve steel performance and reduce experimental costs by exploring processing, microstructure, and properties**

The **OCAS** research centre is a joint venture between steelmaker **ArcelorMittal** and the Flemish regional government. OCAS aims to improve steel properties by gaining a detailed understanding of the many subtle relationships that drive steel properties. This project investigated the application of machine learning to this task. Even minor improvements in steel performance or in the cost of raw materials and processing can drive enormous economic benefits. OCAS is also seeking insights that can reduce the amount of costly and time-consuming physical experiment and analysis required to achieve these results.

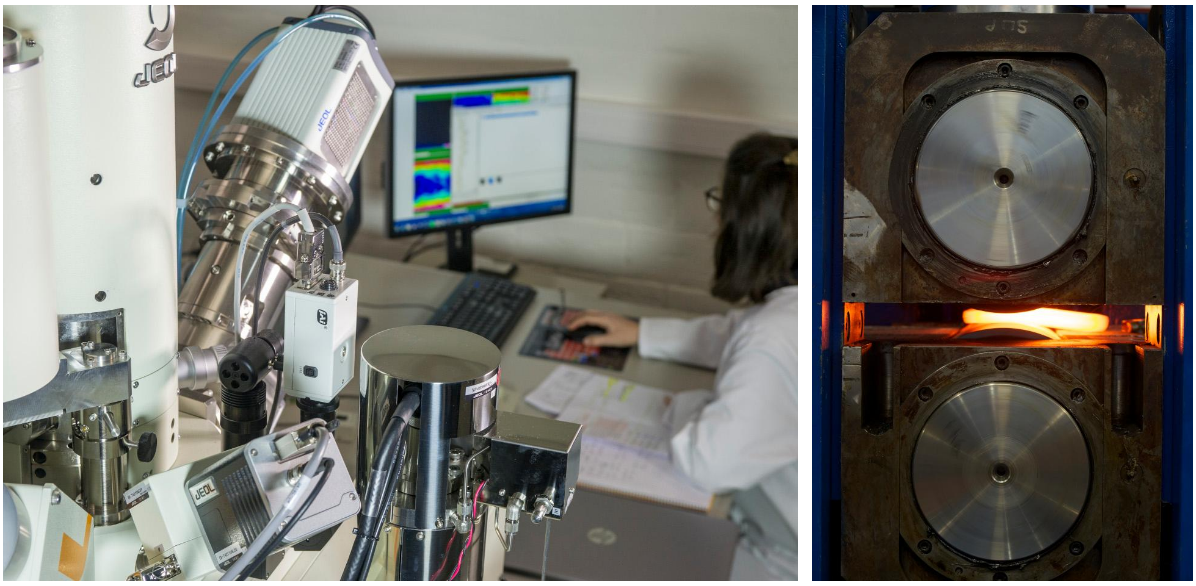

Figure 1. Microscopy (left) and a rolling process (right) at OCAS.

The project aimed to leverage microstructural imaging information to explore the so-called 'PSP triangle' (Processing - Structure - Properties) for steels. Steel microstructures are a treasure trove of information that could be exploited via machine learning.

The solution

The project applied the Alchemite™ deep learning software [1] from Intellegens. Alchemite™ has been designed for use in materials research and development, with key features being its ability to generate machine learning models from real-world, sparse, noisy experimental data, and the accuracy with which it quantifies the uncertainty associated with its predictions.

Alchemite™ was trained on an OCAS steel dataset. The data consisted of four material chemistries, 23 unique treatments, nine processing variables, and microstructural image data. Microstructures were encoded for Alchemite™ using a combination of deep learning and principal components analysis.

The project analysed microstructure image data along with process and property data

The project investigated the accuracy of the machine learning model, and how it varied when trained using different combinations of image, process, and property data. The aims of this exercise included understanding the impact of image magnification on the accuracy of predictions, and establishing how sensitive the predictions were to different parts of the dataset.

Such understanding provides insight into the 'PSP' relationships, by exposing salient predictors identified by the machine learning model, as well as uncovering their interdependencies. Such an approach could save future effort, time, and cost by enabling more focused testing on the data that is most useful for predicting steel behaviour.

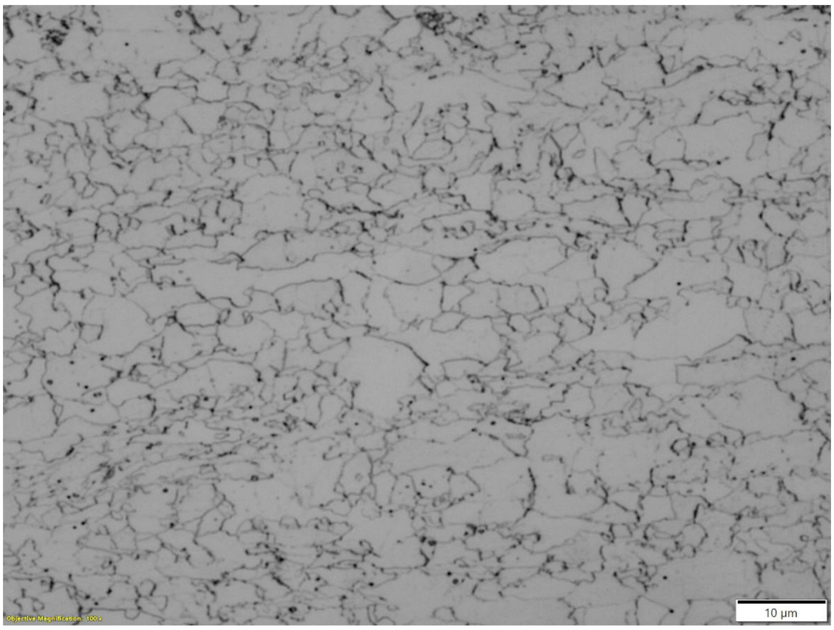

Figure 2. Sample microstructure image from the project.

Finally, after model assessment, Alchemite™ was used to optimise experimental processing parameters in order to identify a combination of inputs that best met specific property requirements for the steels.

Outcomes

> **Alchemite™ was able to build accurate models and provide insights that could reduce future experimental workloads**

- Alchemite™ was able to build models which demonstrated good accuracy (R^2 values > 0.8) in property prediction. Accuracy was improved by including microstructure image data.
- When using microstructure images at one particular magnification as input, model accuracy was better than with images at other magnifications. This suggests that features which resolve at this magnification are most significant, and may enable the range of images captured in future tests to be reduced, saving time and cost.
- In some circumstances, it was possible to remove up to 30% of the image data without significantly impacting model accuracy. Again, this suggests that, while microstructure data enriches the model, not every sample needs to be imaged, with resulting cost savings.
- The project developed an understanding of the importance of including processing and/or microstructural data in different circumstances, e.g., when interpolating within the range of existing experiments versus extrapolating beyond this range.
- 'Explainable AI' tools helped to understand which specific inputs were most useful in predicting performance. One example, a sensitivity plot, is shown in Figure 3.
- Alchemite™ was able to design a set of processing parameters to achieve target properties for the steel.

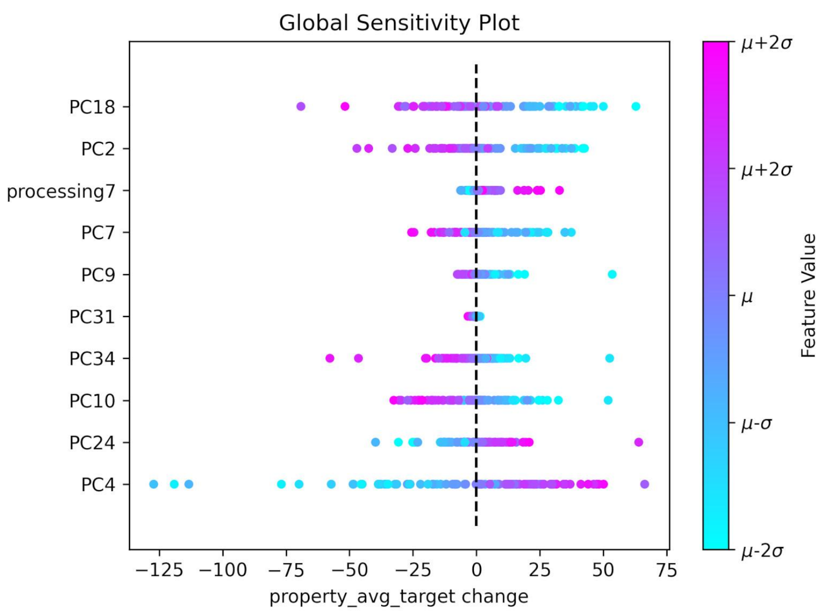

Figure 3. Global sensitivity plot - an 'explainable AI' tool in Alchemite™. The plot enables the overall impact of each variable on the target property to be assessed.

Summary

The OCAS project team assessed the benefits of the project as:

- Alchemite™ deep learning allows extraction of hidden information from microstructural images.
- Alchemite™ provides models with good predictive power, going from processing and /or microstructure to properties.
- The model becomes less of a 'black box' when supported by analytics features, such as importance charts and sensitivity plots, and through providing reliable uncertainty estimates on predictions.
- The ability to deal with sparse and noisy data is essential for extracting useful information out of real-world datasets.

Lode Duprez, chief scientific officer at OCAS, commented:

"The project has validated the use of the deep learning method for real–world steels applications and provided us with insights that can help us to improve steel properties and focus valuable experimental resources more efficiently. We found the feature importance and sensitivity plots to be a very worthwhile guide."

About OCAS and Intellegens

OCAS NV is a research centre of Finocas, a joint venture between the Flemish region and global steel leader **ArcelorMittal**. OCAS provides steel and metal-based products, services, and solutions to metal processing companies worldwide. OCAS develops alloys and coatings, produces and tests samples, and co-develops steel applications. With over 150 researchers and engineers, it is equipped with state-of-the-art R&D tools and facilities in its laboratories in Zelzate and Zwijnaarde (Belgium).

Intellegens provides unique deep learning software, Alchemite™. Our focus is on making it easy to apply machine learning to accelerate innovation in materials, chemicals, manufacturing, and beyond. Alchemite™ can train machine learning models from real-world, sparse, noisy data. The method originated at the University of Cambridge and development is on-going at Intellegens. Successful applications include industrial R&D and process improvements in superalloys, additive manufacturing, chemical processes, formulated products, batteries, and drug discovery.

References

1. "Alchemite™ deep learning - solving complex problems with real-world data", *Intellegens White Paper* (2021)

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