Machine Learning based Prediction of the Martensite Start Temperature

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Introduction

The martensite start temperature (Ms) is used for the optimization of the heat treatment of steels and to tailor its microstructure and its mechanical properties such as hardness, toughness, strength and ductility by precisely controlling the formation and amount of martensite. The Ms mainly depends on the chemical composition, but still is a complex problem to predict. Previous works applied empirical [1], machine learning [2, 3] and thermodynamic [4] models successfully within limitations, such as focus on certain steel types or by executing additional feature engineering. The goal of this work is to overcome existing limitations and improve the Ms prediction accuracy for all steel types in a single machine learning model.

Method

Two publicly available datasets [4, 5] were merged and cleaned, retrieving a total of around 1800 entries with up to 15 chemical elements including all types of steel alloys. The Ms ranges from 150 K to 790 K, but is imbalanced having substantially more Ms above 400 K (s. Figure 2). The training-validation dataset was formed of 1500 randomly selected entries. The remaining 300 entries form the final test dataset. Extensive hyperparameter tuning was performed to find the best multilayer perceptron model (MLP) for this dataset. These included width and depth of the model as well as varying optimizers, activation functions, momentum, weight decay and learning rate. Each model was evaluated using a 5-fold cross validation approach. Finally, the best hyperparameters were trained without cross validation and validated against the test dataset.

Additionally, the explainable AI method SHAP [6], based on shapley values (game-theoretical approach), was applied to estimate the effect of a single chemical element on the Ms in the trained MLP. The goal is to better understand the model's inner workings by calculating the predictions for all possible subsets for a set of chemical elements and compare the differences.

Ms Prediction App

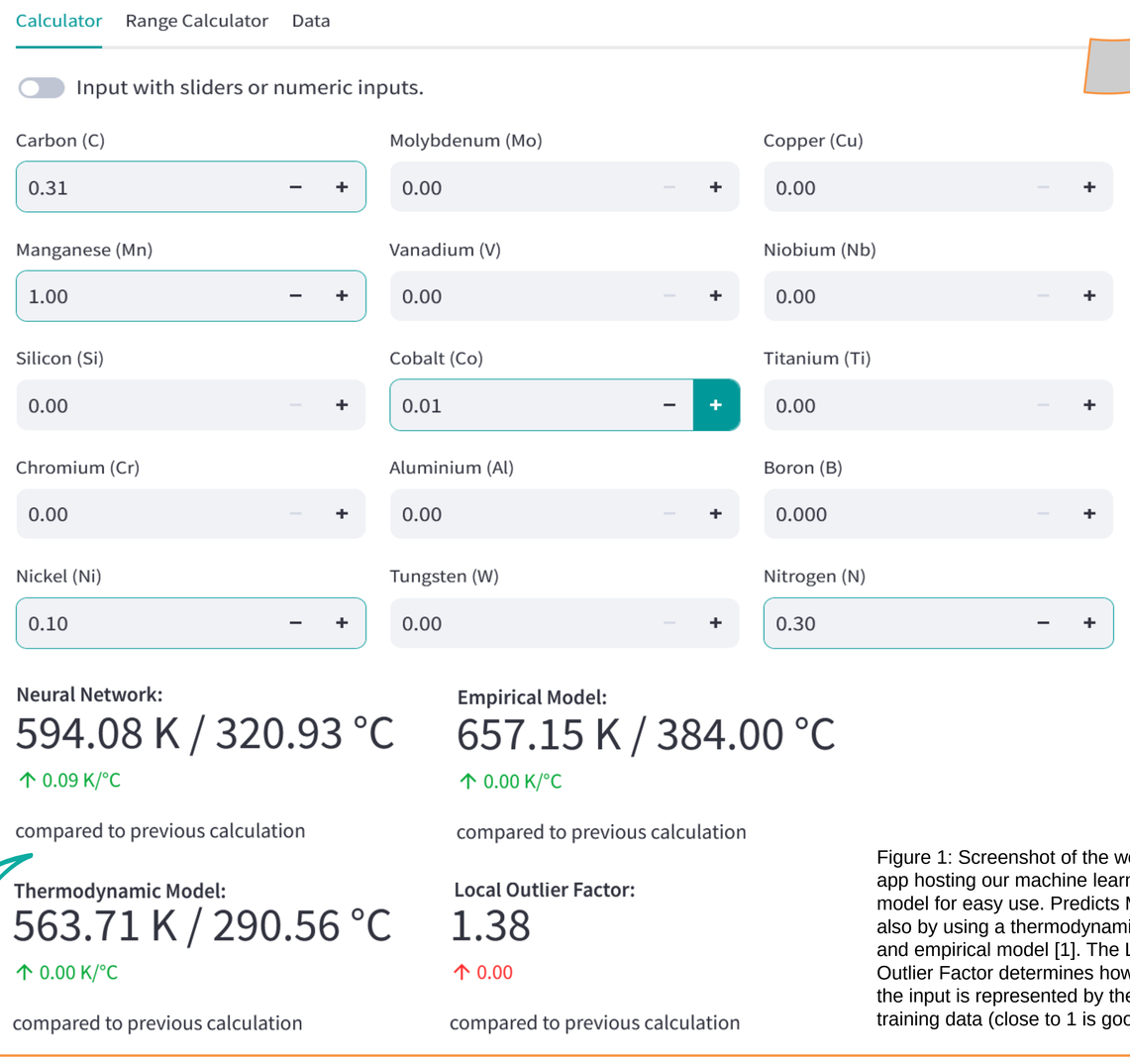
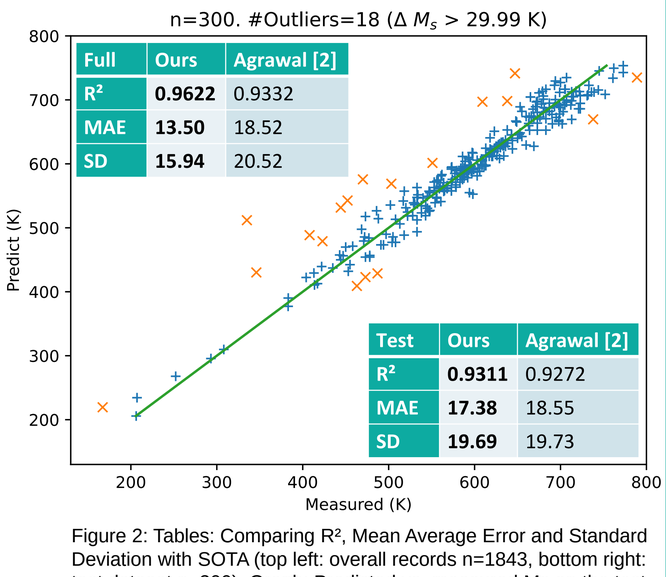


Figure 1: Screenshot of the web app hosting our machine learning model for easy use. Predicts Ms also by using a thermodynamic and empirical model [1]. The Local Outlier Factor determines how well the input is represented by the training data (close to 1 is good).

Results

The best MLP consists of two hidden layers, 64 parameters each, with a total of 5000 trainable parameters. It outperforms the existing state of the art model [2] as displayed in Figure 2. Also, two outliers were found that the model could not fit well, but no other model could fit them well either.

The final model is deployed as Web App which can be seen in Figure 1. The SHAP analysis in Figure 3 shows the average impact for each element on the prediction of the Ms.



Full	Ours	Agrawal [2]
R^2	**0.9622**	0.9332
MAE	**13.50**	18.52
SD	**15.94**	20.52

Test	Ours	Agrawal [2]
R^2	**0.9311**	0.9272
MAE	**17.38**	18.55
SD	**19.69**	19.73

Figure 2: Tables: Comparing R^2, Mean Average Error and Standard Deviation with SOTA (top left: overall records n=1843, bottom right: test dataset n=300). Graph: Predicted vs. measured Ms on the test dataset, orange „x" marks outliers (Δ> 2σ as of training dataset).

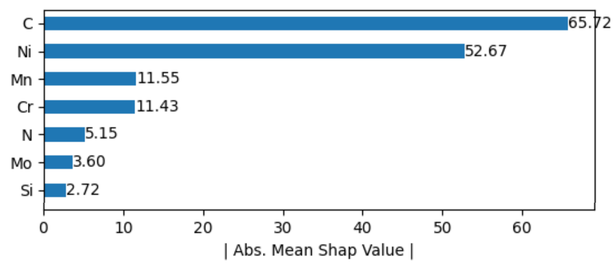


Figure 3: Average impact of element as calculated by SHAP.

Further analysis showed that these values vary considerably, depending on the actual alloy. Yet, according to our model both C and Ni have the greatest impact, while Mn, Cr and N have a similar medium impact.

Conclusion

This work presents

i) a deep learning model for the prediction of Ms which
ii) achieves higher overall accuracy than existing models while
iii) not being restricted to certain steel types, removing the need-to-know which model predicts best for a certain steel alloy.

The model is not explicitly constrained to physically meaningful values and may predict a Ms below 0 K. A physics-constrained network could potentially overcome these effects. (More) Publicly available data in high quality helps building better models, but carefully examining them for unrealistic data is important too. Grain size and cooling rate have not been considered. The prediction can still be improved for steels that are not yet part of the training data.

Explainable AI methods like SHAP help to understand the inner workings of the model, but not yet the physics.

References

[1] Ingber, Kunert (2021). Prediction of the Martensite Start Temperature in High-Carbon Steels. Steel research international. 93(5), p. 2100576.
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[4] Palumbo (2008). Thermodynamics of martensitic transformations in the framework of the CALPHAD approach. Calphad. 32(4), p. 693–708.
[5] Sourmail and Mateo (2004). Map martensite start temperature data library. URL: https://www.phase-trans.msm.cam.ac.uk/map/data/materials/Ms_data_2004.html (Accessed 17.10.2023)
[6] Lundberg and Lee (2017). A Unified Approach to Interpreting Model Predictions. Proceedings of the 31st International Conference on Neural Information Processing Systems, p. 4768-4777.

Open Source

Access the App via the QR-Code above or:
https://eah-jena-ms-predictor.streamlit.app

Newly formed Database and Source code
are available at:
https://github.com/EAH-Materials/MartensiteStart_DeepLearning

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