Development of Microstructural Evolution Models for Hot Rolling Integrating Advanced Numerical Tools

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Keywords: hot rolling; microstructural modeling; hybrid models; Artificial Intelligence

INTRODUCTION

The accurate prediction of microstructural evolution during hot rolling is critical for achieving target mechanical properties, optimizing process parameters, and ensuring product consistency across varying steel grades and mill configurations. Traditional metallurgical models, grounded in physical mechanisms such as recrystallization, grain growth, and phase transformation kinetics, are instrumental in understanding and simulating hot deformation behavior. However, their applicability is often constrained by the need for extensive calibration and their limited adaptability to new alloy systems or process routes. This study introduces a novel hybrid modeling framework that integrates physically-based metallurgical models with advanced numerical tools and data-driven methodologies, including Artificial Intelligence (AI) techniques. The core of this framework is built upon a suite of in-house modeling tools: MicroSim, for austenite evolution; PhasTranSim, for phase transformation; and MechPropSim, for mechanical property prediction. These models are designed to interact with industrial rolling schedules, capturing complex thermomechanical histories and their influence on final product characteristics.

A key innovation of the MicroSim model is its capability to simulate the evolution of full austenite grain size distributions, rather than mean values, allowing for a more realistic representation of inhomogeneities (both local and through-thickness) driven by thermal and strain gradients. This feature is particularly relevant for plate rolling and thick sections, where gradient effects are significant. MicroSim has been developed to support a wide range of hot rolling lines, including Plate Mills, Hot Strip Mills, Steckel Mills, and long product mills (bars, H-Beams and sections). Recent developments include the integration of PhasTranSim, which predicts phase fractions and transformation kinetics during cooling, and MechPropSim, which estimates mechanical properties based on microstructure and composition. In this work, MechPropSim is further enhanced using symbolic regression algorithms to derive empirical models that link process variables and microstructural features to yield strength, enabling greater transparency and transferability compared to traditional black-box machine learning approaches. This hybrid modeling approach offers a pathway to intelligent and adaptive rolling mill operations.

By embedding advanced models into production environments, the framework facilitates predictive control, real-time quality assurance, and energy-efficient process design. The convergence of metallurgical knowledge and AI techniques enables robust and scalable solutions for modern steelmaking, aligned with the industry's increasing emphasis on digitalization, sustainability, and process optimization.

MICROSTRUCTURAL EVOLUTION MODELING

The core structure of the modeling framework is built around the MicroSim and PhasTranSim models, supported by an integrated thermal module. Together, they enable a detailed simulation of the austenite conditioning during rolling and the subsequent phase transformations during cooling, offering a powerful tool for both process optimization and alloy design. In Figure 1, the different blocks of the hot rolling modeling software are visualized. The first block, MicroSim, is responsible for predicting the evolution of austenite during the process. For this prediction, an initial distribution of austenite grain sizes is used, and the microstructural evolution of the different bins in the distribution is considered. The next block, PhasTranSim, involves phase transformation calculations. This block calculates when phase transformations occur and outputs the grain size and fractions of resulting constituents such as ferrite, pearlite, bainite and/or martensite. Finally, the latest addition to the

software is MechPropSim, which predicts the mechanical properties of the final product, such as tensile strength (TS) and yield strength (YS), based on a metallurgical model accounting for each individual strengthening contribution.

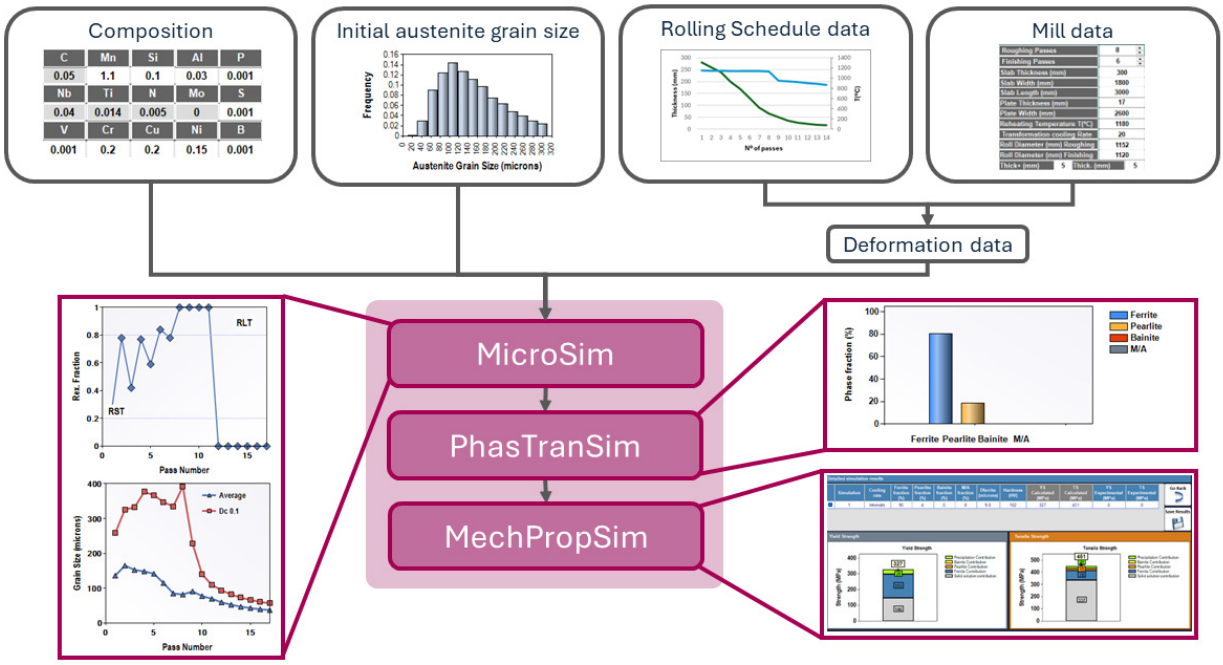


Figure 1. Schematics of the MicroSim, PhasTranSim and MechPropSim modules and input/output information.

MicroSim is designed to simulate the evolution of the austenite grain structure under industrial rolling conditions. Unlike conventional models that rely on mean grain size values, MicroSim computes the evolution of full grain size distributions by discretizing the microstructure into grain size bins. Each bin evolves independently according to local strain, temperature, and time histories, enabling the model to capture the heterogeneity typical of industrial rolling, especially in thick plates where through-thickness gradients are pronounced [1]. The model accounts for the main microstructural mechanisms that govern austenite evolution: dynamic recrystallization is modeled as a strain-dependent process, influenced by strain rate and temperature, while static and metadynamic recrystallization are treated as time-temperature transformations affected by solute drag and precipitation effects. In microalloyed steels, strain-induced precipitation plays a particularly relevant role by retarding recrystallization during finishing passes, which leads to a pancaked austenite structure and refined transformation products. The evolution of precipitates and their effect on recrystallization is therefore integrated into the model linked to composition and deformation parameters.

The thermal model embedded within MicroSim enables the prediction of through-thickness temperature profiles, using rolling conditions to reconstruct internal gradients. This allows for the evaluation of local temperatures at different depths—surface, quarter-thickness, and centerline—and their influence on recrystallization, strain accumulation, and grain size evolution. When combined with the MicroSim calculations, this model offers a comprehensive view of through-thickness microstructural heterogeneity and its relationship to rolling and cooling strategies [2].

Following the austenite evolution, the transformation to ferrite, pearlite, bainite, or martensite during cooling is modeled using PhasTranSim. This model takes the output from MicroSim—specifically the final austenite grain size distribution, degree of pancaking, and chemical composition—as initial conditions to predict the kinetics of phase transformations. Ferrite formation is modeled based on nucleation at prior austenite grain boundaries, with transformation kinetics strongly influenced by grain refinement and prior strain history. The model uses time-temperature-transformation concepts adapted to continuous cooling paths, considering the effects of composition and grain size on transformation start times and phase fractions. In the case of martensitic transformation, the model uses established relationships to estimate the martensite start temperature (M_s) and resulting hardness, based on the alloying content and the austenite microstructure.

The integration of MicroSim, PhasTranSim, and the thermal model enables end-to-end simulation of microstructure development from reheating to final cooling. This framework has been applied to a variety of industrial use cases involving Nb, Ti, and Mo microalloyed steels, demonstrating its capability to reproduce the influence of reheating temperature, strain path, interpass times, and cooling rate on both microstructural evolution and final mechanical response. The models have proven particularly useful in understanding through-thickness heterogeneity in thick plates, validating temperature models via

Mean Flow Stress analysis, and evaluating transformation behavior using predicted cooling curves and transformation start times.

MechPropSim module, currently under development, predicts yield (YS) and tensile (TS) strengths based on a metallurgically based model. It is well reported that the yield strength of low carbon microalloyed steels can be described as a combination of different strengthening contributions. The initial approach in MechPropSim was set on a linear approach based on the sum of the contributions (solid solution [3], grain size [4], dislocations [5], and fine precipitation [6]) (Equation (1)). To estimate the individual contributions, equations previously reported in the literature were employed and a more detailed description of the expressions and symbols can be found in [7,8].

$$\sigma_y = \sigma_0 + \sigma_{ss} + \sigma_{gs} + \sigma_\rho + \sigma_{ppt} \quad (1)$$

After an initial validation step, it was observed that individual strengthening contribution predictions were not very accurate when compared to measurement-based estimations resulting from the above references papers. Therefore, a more advanced prediction tool based on artificial intelligence was developed and this is the core development described in the following section.

ADVANCED MATHEMATICAL TOOLS

While physically-based microstructural models such as MicroSim and PhasTranSim provide a robust foundation for understanding the underlying mechanisms of hot deformation and phase transformations, their predictive capability can be further enhanced through the integration of data-driven approaches. In particular, the application of symbolic regression techniques introduces a complementary modeling strategy capable of capturing complex, non-linear relationships between process variables, microstructure, and mechanical properties. This hybrid approach leverages the explanatory power of physical metallurgy of AI-based methods to extract interpretable equations from experimental and industrial data. In this work, symbolic regression is employed to develop empirical models that enrich the existing microstructural modeling framework, focusing on critical aspects such as ferrite grain size, dislocation density, and yield strength. These models are trained using experimental datasets and process outputs from MicroSim and PhasTranSim, forming a bridge between simulation-driven insights and data-derived correlations. The integration of symbolic regression thus represents a step forward in creating intelligent, self-adaptive models that enhance both accuracy and interpretability in rolling process predictions. The expansion of these advanced tools is ongoing for other modules such as Mean Flow Stress predictions and microalloying element solubility estimations.

Symbolic Regression

Symbolic regression (SR) is an Artificial Intelligence method that searches for a model in the form of a symbolic equation, combining mathematical functions to fit a set of data. SR can be a useful tool for discovering empirical equations and provides an output that is easily interpretable. Although there are many ways to perform the task of searching for equations, the most common approach is to represent equations as trees with operators, variables, or parameters as nodes and to use genetic algorithms for optimization [9]. The main objective is to find an equation that is as simple as possible while maintaining proper accuracy.

One of the main challenges in the materials field is the limitation of data, especially when it needs to be obtained through experimental tests. The smaller the dataset, the higher the error, and the greater the degree of freedom required in the model to improve accuracy [10]. Symbolic regression can be used to develop models for small datasets and is effective at generalizing beyond the training set [11].

In this study, PySR software was selected for SR training due to its flexibility in creating custom problems and its superior performance compared to other software in many aspects [99]. The objective is to evaluate the viability of symbolic regression for hot rolling modeling. Consequently, all models were developed using PySR's default settings, utilizing the operators ["+", "*", "-", "/", "^"]. A constraint was applied to the "^" operator, limiting the exponent to a maximum complexity of one.

SR Applied to Mechanical Properties Prediction

For mechanical properties prediction, data-driven models are becoming increasingly popular [12]. Mechanical properties can be measured in plants, and these, along with other process parameters, can be used to train robust machine learning algorithms. However, these algorithms are often not transferable between plants or require retraining when a new product is manufactured. This study aims to develop a mechanical properties model that is applicable to different products and provides insights into the strengthening mechanisms involved.

Previously, MechPropSim relied on empirical models from the literature to calculate mechanical properties, specifically yield strength. However, this approach did not yield the expected results, and the model was not sufficiently accurate. Therefore, this study focuses on improving the block's accuracy by employing a hybrid method that combines well-known expressions from

the literature with a symbolic regression algorithm. This approach aims to produce a model that is both accurate and informative about the strengthening mechanisms in the alloy and process.

To train the model, a dataset of 20 samples from multiple plate mill plants was used. This dataset includes industrial rolling data, composition, mechanical properties, and additional laboratory measurements of the microstructure. Contributions from the previous MechPropSim model were also incorporated, calculated using literature formulas with the precipitation contribution determined as the remainder of the total YS value.

However, to enable MechPropSim use in an online process, certain variables that are not directly measurable must be calculated as part of PhasTranSim. Specifically, this includes the ferrite grain size and dislocation density. Consequently, three models were developed: one for predicting ferrite grain size, another for dislocation density prediction, and one for yield strength.

Ferrite Grain Size

Symbolic regression has been applied to derive empirical expressions for ferrite grain size. Low angle boundary unit size values were selected in this case, as this magnitude is affecting the yield strength properties. Both process parameters and results from MicroSim are utilized in this model. In line with the understanding of ferrite grain size, symbolic regression searches for an equation in the form of f(CR, Dγ, C, Mn, Mo, V, Nbsol). Figure 2 shows the Mean Absolute Error (MAE) of the training and test samples as a function of equation complexity, compared with the previous model used in the software.

Expressions with low complexity, such as a constant or a binary operation between two variables, are not complex enough to accurately represent the mechanisms. Conversely, when the complexity is too high, the algorithm's performance also deteriorates. Thus, an equation with a complexity around 9 appears to be the best option. When compared to the previous predictions, it is evident that although the error remains high in some cases, the improvement over the previous model is significant.

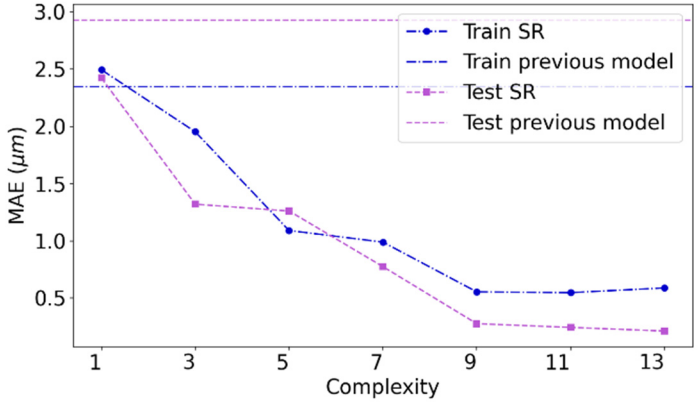


Figure 2. MAE values for ferrite grain size prediction as a function of equation complexity.

Figure 3 presents the predicted values compared with the actual measurements for the selected best model. In this case, the model with complexity 9 was selected as the best due to its low MAE value. Increasing the complexity would result in reduced interpretability without significantly improving the error. It is evident that, for both the training and test sets, the symbolic regression models with relatively high complexities closely match the measurements.

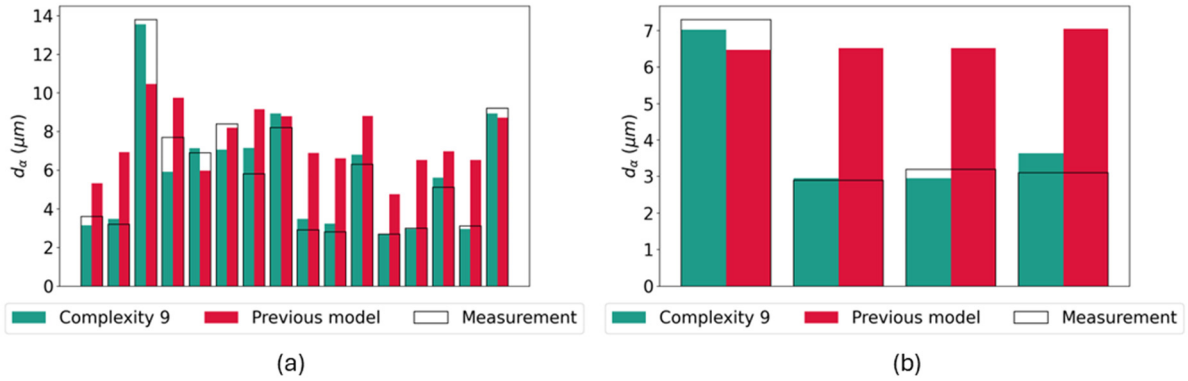


Figure 3. Comparison between ferrite grain size measurements with predictions from previous model and the selected SR model. (a) Training set; (b) Test set.

Dislocation Density

To model the dislocation density, estimated using the Kernel Average Misorientation (KAM) values measured by EBSD [5], symbolic regression is used to search for a function in the form of f(CR, C, Mo, Nbsol). Figure 4 presents the MAE versus complexity. No previous model is available for comparison, as predicted dislocation density was not included in earlier versions of the model. It is observed that low-complexity models exhibit high errors, while complexities between 5 and 9 yield good results. For equations with higher complexities, the errors begin to stabilize, making further increases in complexity unnecessary.

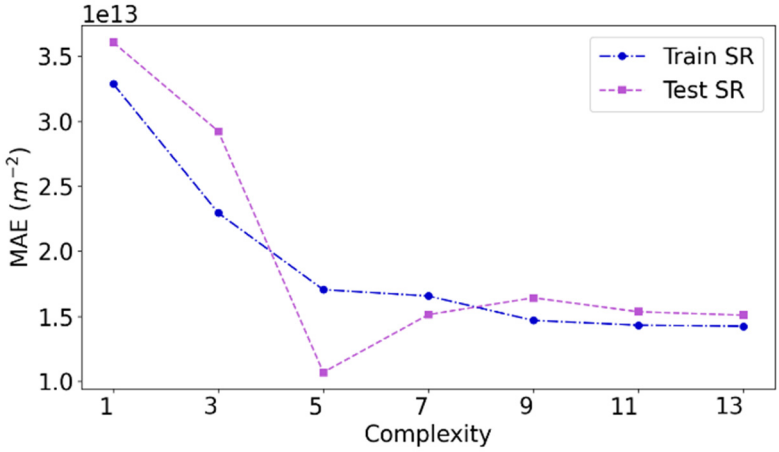


Figure 4. MAE values for dislocation density prediction as a function of equation complexity.

Figure 5 displays the real measurements alongside the predicted values from the complexity 9 model. This model was selected because it offers a good trade-off between error and complexity based on the training set. In most cases, the predictions closely match the measurements. Although there are some exceptions where neither model performs well, the errors remain close to the measurement error.

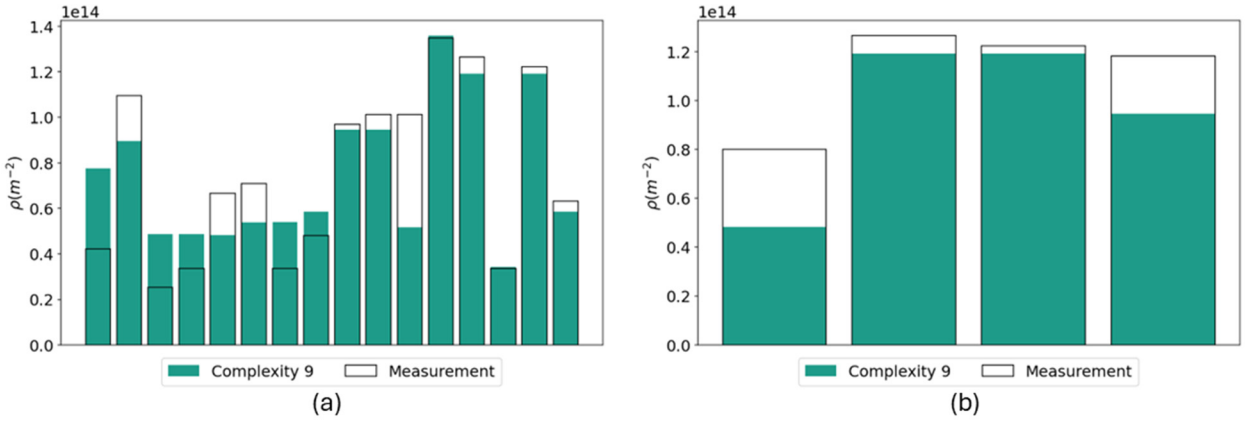


Figure 5. Comparison between dislocation density predictions from previous model and the selected SR model. (a) Training set; (b) Test set.

Yield Strength Predictions

As previously mentioned, the modeling of yield strength has been extensively studied. The aim here is to develop a hybrid model using symbolic regression to derive an equation that integrates existing knowledge. The expression in Equation (1) outlines the yield strength contributions considered in this study. As mentioned before, several of these contributions are well-documented in the literature. For instance, the yield strength of iron is typically around 53.9 MPa, and the influence of ferrite grain size follows a relationship proportional to $d_{\alpha}^{-0.5}$. In the case of solid solution strengthening, various formulas exist; here, this contribution is treated as a function $f(Mn,\ Si,\ Mo,\ N_{free})$, which will be determined using symbolic regression. The contribution from dislocation density generally exhibits a direct proportionality to $\rho^{0.5}$. Similarly, for precipitation strengthening, and due to the lack of accurate volume fraction measurement, there was no individual contribution validation. So, this contribution will also be derived through SR as a function $f(C \cdot \mathrm{V}, \mathrm{N_{free}} \cdot \mathrm{V},\ \mathrm{C} \cdot \mathrm{Nb_{sol}}, \mathrm{C} \cdot \mathrm{Ti_{eff}},\ \mathrm{CR})$.

Also, it is worth mentioning that the loss function is constructed to minimize the error between the predicted total yield strength and the measured values. Additionally, the loss function includes terms to minimize the deviation of each contribution from the corresponding values in the dataset from the previous study.

Figure 6 shows the MAE versus the complexity of the σ_{ss} and σ_{ppt} terms, where symbolic regression is used to discover equations. The MAE of the training and test sets from the previous model is used for comparison. It is evident that the equations obtained require very low complexity for these two terms, with a complexity of 4 being sufficient. This is reasonable because this level of complexity accounts for only two terms, whereas the complexity of the full yield strength expression is much higher. Additionally, having a high complexity would not be practical, given that only 16 samples are used for training.

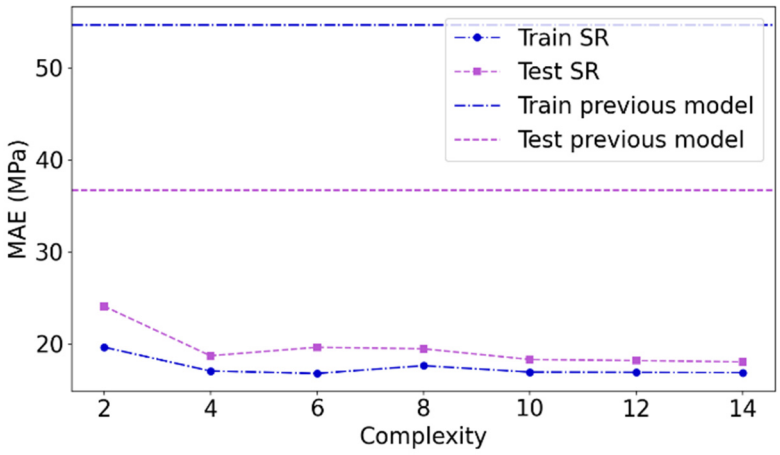


Figure 6 MAE values for yield strength prediction as a function of equation complexity.

Figure 7 displays the measured and predicted values for complexity 4 model, which has been found to be sufficient for modeling the yield strength. It is evident that the model obtained through symbolic regression is in good agreement with the measurements. While the previous model performs well and even better in some samples, it exhibited unacceptable errors in others. In contrast, the symbolic regression approach accurately predicts all samples.

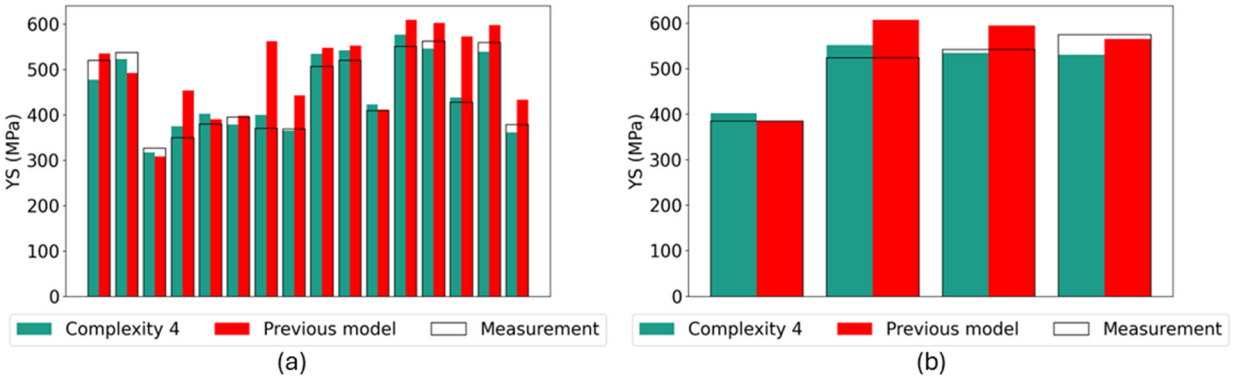


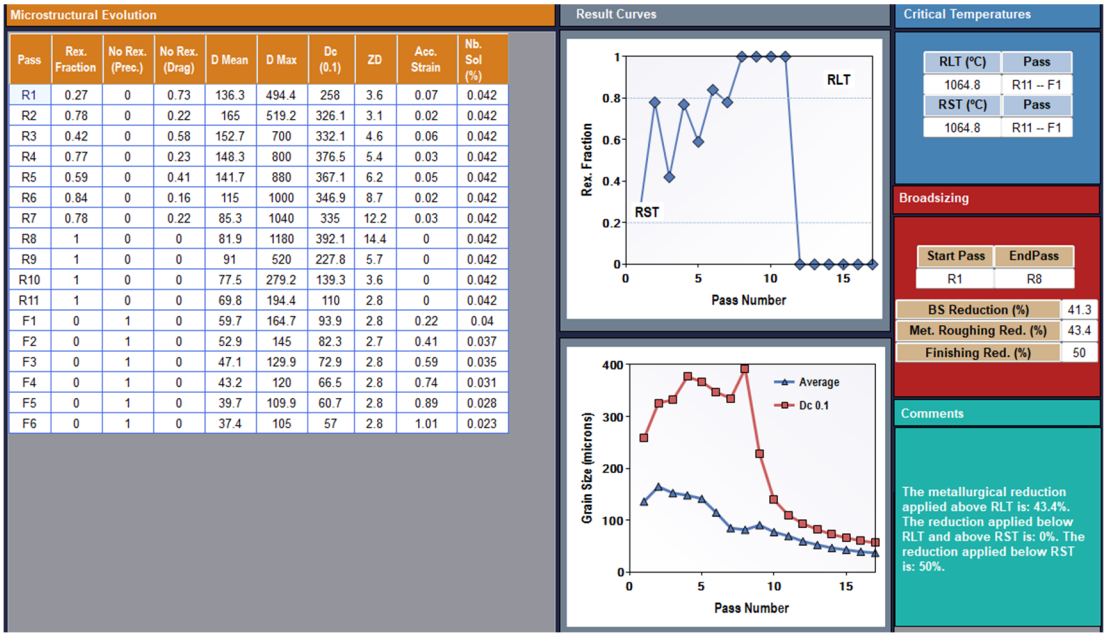
Figure 7 Comparison between yield strength measurements with predictions from previous model and the selected SR model. (a) Training set; (b) Test set.

From the results presented in this section, SR can be an interesting approach for improving individual strengthening contributions as well as predicting YS values within a reliable range. As this work progresses, and additional data sets are included into the training set, new expressions with a higher validity for a wider interval of chemical compositions and processing conditions will be recalculated. The same approach is also ongoing for coiled strip products where, in addition to rolling and runout table cooling conditions, the effect of coiling must be considered in the prediction of mechanical properties.

MODEL APPLICATION FOR THE PRODUCTION OF A NB-TI 50 MM THICK PLATE

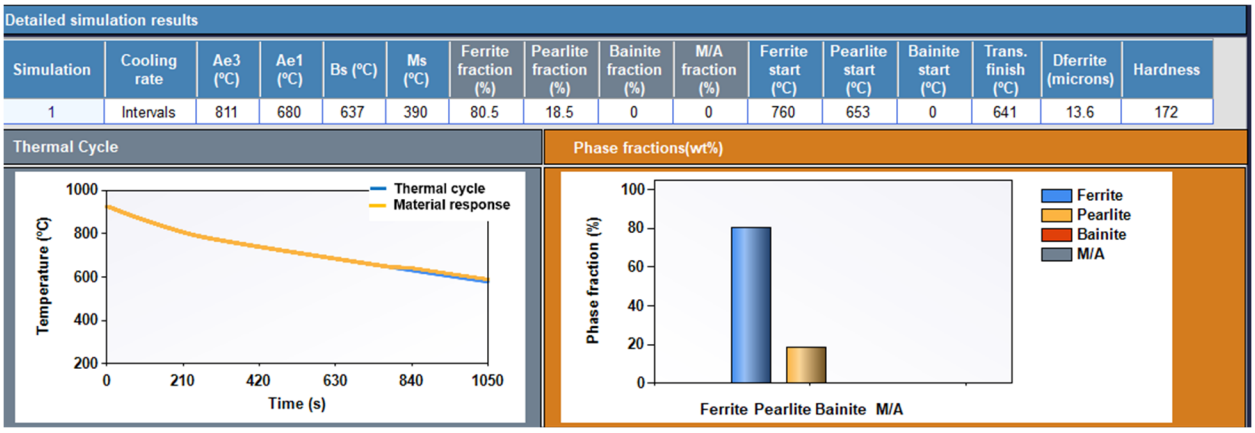
The above describe model was applied to the hot rolling of an air-cooled 50 mm thick plate. The chemistry was defined as a S355 grade 0.16%C, 1.5%Mn steel microalloyed with 0.04%Nb and 0.02%Ti. The rolling schedule was defined as a combination of 11 roughing passes and 6 finishing passes, after a reheating at 1250ºC and a finish rolling temperature of 925ºC. Figure 8 shows the results from MicroSim Plate Mill model. Using the Temperature Model, the cooling path after the last

finishing pass was calculated using air cooling conditions without any accelerate cooling step. The equivalent cooling rate calculated in the 800-500ºC range is of 0.3ºC/s in the quarter position of the plate. PhasTranSim model results (see Figure 9) show a phase balance of about 80% ferrite, 20% pearlite combination in the final microstructure. The measurements in the industrially processed plate resulted in a fraction of 75% ferrite and 25% pearlite and a Vickers Hardness of 172.2 HV, very close to the values predicted by PhasTranSim. The ferrite grain size measured in the optical microscope results in an average grain size of 10 µm, lower than the one predicted by PhasTranSim. In the current PhasTranSim version, the prediction for grain size is limited to polygonal ferrite structures and provides values of high angle boundary unit sizes. This value will be different for the mechanical property model where a low angle boundary unit size is predicted and considered for the strengthening contribution. This change will help to better predict non-polygonal or acicular type of microstructures.



Pass	Rex. Fraction	No Rex. (Prec.)	No Rex. (Drag)	D Mean	D Max	Dc (0.1)	ZD	Acc. Strain	Nb. Sol (%)
R1	0.27	0	0.73	136.3	494.4	258	3.6	0.07	0.042
R2	0.78	0	0.22	165	519.2	326.1	3.1	0.02	0.042
R3	0.42	0	0.58	152.7	700	332.1	4.6	0.06	0.042
R4	0.77	0	0.23	148.3	800	376.5	5.4	0.03	0.042
R5	0.59	0	0.41	141.7	880	367.1	6.2	0.05	0.042
R6	0.84	0	0.16	115	1000	346.9	8.7	0.02	0.042
R7	0.78	0	0.22	85.3	1040	335	12.2	0.03	0.042
R8	1	0	0	81.9	1180	392.1	14.4	0	0.042
R9	1	0	0	91	520	227.8	5.7	0	0.042
R10	1	0	0	77.5	279.2	139.3	3.6	0	0.042
R11	1	0	0	69.8	194.4	110	2.8	0	0.042
F1	0	1	0	59.7	164.7	93.9	2.8	0.22	0.04
F2	0	1	0	52.9	145	82.3	2.7	0.41	0.037
F3	0	1	0	47.1	129.9	72.9	2.8	0.59	0.035
F4	0	1	0	43.2	120	66.5	2.8	0.74	0.031
F5	0	1	0	39.7	109.9	60.7	2.8	0.89	0.028
F6	0	1	0	37.4	105	57	2.8	1.01	0.023

Figure 8. MicroSim results for the 50 mm hot rolled plate.



Simulation	Cooling rate	Ae3 (ºC)	Ae1 (ºC)	Bs (ºC)	Ms (ºC)	Ferrite fraction (%)	Pearlite fraction (%)	Bainite fraction (%)	M/A fraction (%)	Ferrite start (ºC)	Pearlite start (ºC)	Bainite start (ºC)	Trans. finish (ºC)	Dferrite (microns)	Hardness
1	Intervals	811	680	637	390	80.5	18.5	0	0	760	653	0	641	13.6	172

Figure 9. PhasTranSim results for the 50 mm air-cooled plate.

Using these new submodels as the prediction engine for the MechPropSim model, an YS of 438 MPa is predicted, while the measured YS is of 428MPa. Figure 10 shows the different strengthening contributions to reach these properties. It is important to note that, while the total yield strength value in the expert estimation is a real measurement, the individual mechanism contributions are not directly measured. The contributions are estimated based on EBSD measurements such as low angle boundary unit sizes for grain size and Kernel Average Misorientation for dislocation density. Due to the lack of accurate measurements of precipitate volume fractions, the contribution of fine precipitation (σ_{ppt}) was estimated by subtracting the strengthening associated with all the other contributions from the experimental yield strength. Therefore, the symbolic regression models aim to approximate the total YS value and produce contributions that are consistent with expert assessments, rather than to replicate them exactly. In any case, the results across all complexity levels show good agreement with expectations.

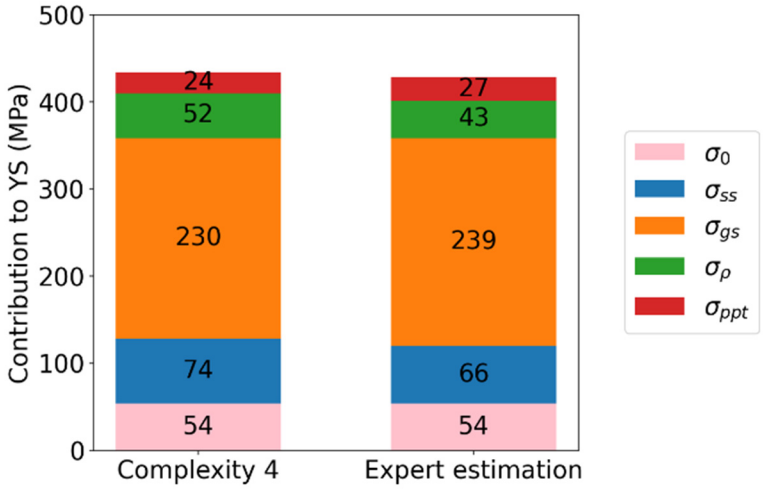


Figure 10. MechPropSim results for the 50 mm hot rolled and air-cooled plate. Comparison between prediction model and experimental expert measurement/estimation.

CONCLUSIONS

This study presents the development and integration of a hybrid modeling framework for predicting microstructural evolution and final mechanical properties in hot rolled steels, combining physically-based metallurgical models with advanced AI-driven tools. The MicroSim and PhasTranSim modules have demonstrated their capability to simulate the evolution of austenite and subsequent phase transformations with high resolution, capturing the influence of composition, strain path, temperature gradients, and microalloying additions on grain refinement and transformation kinetics. By incorporating grain size distributions and through-thickness thermal profiles, the models provide a comprehensive view of the complex interactions occurring during plate rolling.

To complement and extend the predictive power of these models, symbolic regression techniques have been introduced as a data-driven layer capable of extracting interpretable relationships from industrial datasets. The resulting empirical models, applied to ferrite grain size, dislocation density, and yield strength, have shown improved accuracy over traditional formulations while maintaining a physical basis aligned with metallurgical principles. As the training database expands to new plates with broader chemical compositions and processing the conditions, the submodels will evolve to higher accuracy in their predictions. This development is ongoing.

The integration of mechanistic and AI-based approaches within a single modeling platform offers a powerful tool for intelligent process design, virtual alloy development, and adaptive process control in rolling mills. This methodology not only enhances predictive reliability across a broad range of steel grades and processing conditions, but also supports digitalization and sustainability objectives by reducing reliance on plant trials and enabling more efficient, knowledge-based manufacturing strategies.

ACKNOWLEDGEMENTS

The authors acknowledge the financial support provided by the Basque Government through the Elkartek program (ICME-23 Project, KK-2023/00017). Spanish and Basque Governments are also acknowledged for their financial support through the Advanced Functional Materials Program for the New Technological Transformation. Complementary Plan on Advanced Materials 2023–2025. Project no: 101288. Cristina Rodríguez gratefully acknowledges a research grant from the Basque Government (PRE_2024_1_0344).

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