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An AI-Based Approach to Developing a Microstructural Model for Multi-Stage Hot Deformation Processes

Denis Tretyakov[1,a], Nikolay Biba[2,b *], Vitaliy Belugin[1,c], Artur Gartvig[1,d], Andrei Shitikov[1,e] and Sergey Stebunov[1,f]

[1]QForm Group FZ LLC, Fujairah – Creative Tower P.O. Box 4422 Fujairah, UAE

[2]MICAS Simulation Ltd, 107 Oxford Road, Oxford, OX4 2ER, UK

[a]tretyakov.denis.a@gmail.com, [b]nick@qform3d.com, [c]belugin@qform3d.com, [d]gartvig@qform3d.com, [e]a.a.sh.ggml@gmail.com, [f]serg@qform3d.com

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Abstract. Predicting the microstructural state during manufacturing is critical, as it directly governs the material's final mechanical properties. Accurate prediction of microstructure evolution in multi-stage industrial hot deformation processes, such as rolling, is limited by the lack of experimental data at intermediate stages, where direct measurement is impractical. To address this, an integrated methodology combining finite element (FE) simulation in QForm UK® software, physical simulation using the Thermo-Mechanical Treatment Simulator (TMTS), and artificial intelligence (AI) is proposed and investigated.

The methodology is demonstrated for the 11-pass hot rolling of a 41Cr4 steel bar. Thermomechanical loading histories from an FE model of the industrial process were used to design and simulate a targeted TMTS experiment, generating a synthetic dataset via an analytical JMAK model that combines multiple recrystallisation mechanisms. This data was used to train a recurrent neural network (RNN) with an augmented physics-informed Long Short-Term Memory (LSTM) cell to predict the totally recrystallised fraction (RX) solely from loading history data. The AI model achieved high accuracy when validated within the TMTS simulation domain, successfully capturing different recrystallisation regimes. Implementation within commercial FE software enabled direct prediction in the rolling process simulation, yielding promising predictive capability, particularly in regions with thermal histories similar to the training data, highlighting the critical importance of training data diversity.

This work establishes a proof of concept for a novel calibration methodology, where targeted physical simulation bridges the gap between industrial process complexity and data-driven AI model development, offering a practical solution for modelling scenarios where traditional experimental calibration is infeasible.

Introduction

Predicting the microstructural state of a material, or potential micro-defects, is especially challenging for complex multi-step industrial forging or rolling processes [1, 2]. One of the main difficulties is the lack of experimental data for the process's intermediate stages.

For example, in the rolling process, the piece of metal moves continuously from one stand to another, but we have the material's state only at the beginning and end of the whole process. While modelling a single operation, we can assess microstructure, metal flow, and defect formation with quite high accuracy. Sometimes it is even possible to stop forging halfway to observe microstructural development, or to drill channels to visualise material flow. All this provides enough data to calibrate and validate mechanical and microstructural models of a material, or to train corresponding AI models.

In the case of multi-step processes like rolling, AI models could be highly efficient at capturing the dependence of the result on the large number of technological parameters involved. However, the shortage of experimental data needed to train these models is a real bottleneck.

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One solution to this problem could be the development of a methodology and testing equipment capable of reproducing, in laboratory experiments, the most important thermomechanical histories (trajectories) observed in the real multi-step process. This paper is devoted to the proof of concept for this idea.

As an example of a complex technological process, the hot-rolling of a steel round bar on a continuous mill was chosen, and the Thermo-Mechanical Treatment Simulator (TMTS) was selected as the available equipment for simulation experiments.

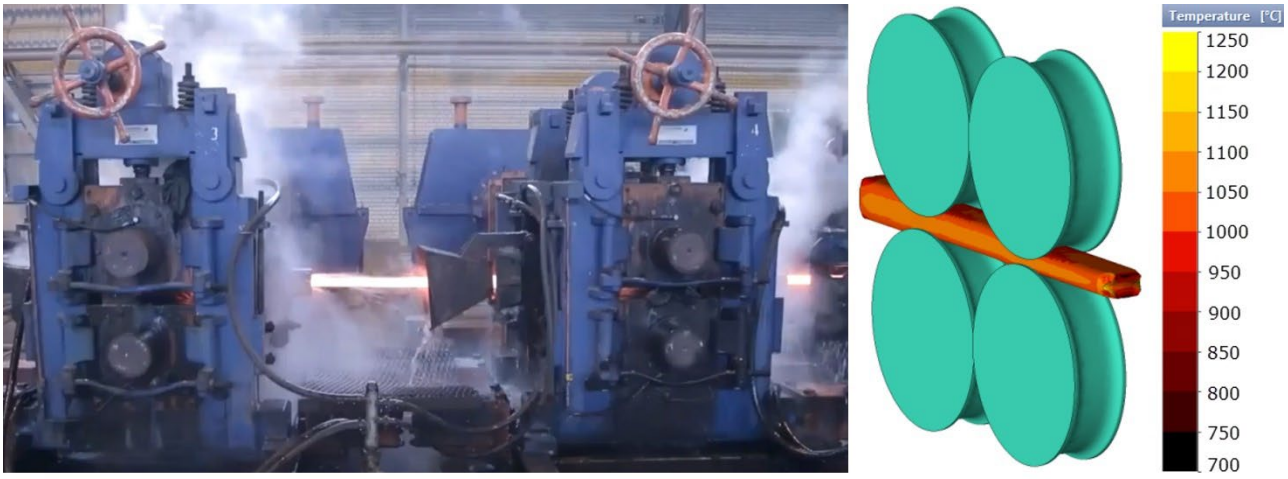
A few conceptual questions were investigated:

1. How is it possible to design an experimental procedure on the TMTS machine capable of imitating the thermomechanical histories of the rolling process?
2. Is the amount, quality, and nature of data obtainable from TMTS experiments suitable and sufficient for training an AI microstructural model?
3. Is an AI microstructural model trained on data obtained from TMTS tests capable of providing reasonable predictions for the real technological process, to what extent and with what limitations?

The investigation of these questions was performed using synthetic data obtained from finite element (FE) simulations of both processes using the commercial metal-forming software QForm UK® and microstructural data simulated using an analytical JMAK-type model. The FE simulation was conducted using the dedicated longitudinal rolling module, as described in [3], which enables full-cycle simulation of a profile rolling process. As for the AI model, a Recurrent Neural Network (RNN) was used with an augmented long short-term memory (LSTM) cell [4], which has previously shown promising results on simpler single-step processes [5] but has been challenging to evaluate on longer, multi-step industrial processes.

Methodology – Hot Rolling

Process description. Hot rolling is a metal forming process where a heated billet is passed through a series of rolling stands to progressively reduce its cross-section and elongate it [6]. In our case, a 100 mm square billet of 41Cr4 steel is rolled into a 28 mm diameter round bar through 11 sequential stands of a continuous mill type 250 (Fig. 1). Each stand consists of grooved rolls that deform the billet, causing a decrease in cross-sectional area known as the draft or reduction and corresponding increases in length (elongation) and width (spreading).



a. b.

Fig. 1. Rolling mill and simulation model: (a) the example of industrial rolling stands during hot deformation of the billet on a continuous mill; (b) corresponding FE representation of the first two stands and billet temperature in simulation.

During each pass, the metal flows to fill the roll groove, and its volume remains approximately constant, aside from minor losses to scale. Thus, reducing the cross-sectional area forces the length

to increase. The elongation coefficient for a pass is defined as the ratio of exit length to entry length. In this 11-pass schedule, the elongation coefficients range roughly from 1.2 to 1.4, meaning the bar's length increases by about 20–40% in each pass. Table 1 summarizes the elongation coefficients, spreading, and absolute reduction for all 11 passes of this rolling process from initial square to final round (Fig. 1b, 2).

Table 1. Rolling reduction schedule for 100 mm to 28 mm bar (11 passes)

Pass No.	Elongation coefficient	Spreading [mm]	Absolute reduction [mm]	Rolling speed [m/s]
1	1.28	11.15	30	0.36
2	1.22	11.71	31.15	0.44
3	1.21	5.57	18	0.53
4	1.26	5.31	15	0.67
5	1.39	13.34	31.59	0.93
6	1.33	12.42	30	1.23
7	1.38	14.19	28.76	1.7
8	1.2	10.24	21	2.05
9	1.34	11.38	21.43	2.74
10	1.21	7.69	15.5	3.32
11	1.32	7.99	15.57	4.37

As the cross-sectional area decreases, the linear speed of the material must increase to maintain constant volume flow through each stand. Throughout the process, the rolls are water-cooled. In the simulation model this roll cooling effect is included as a thermal boundary condition on the roll-workpiece interface to ensure realistic temperature conditions during deformation.

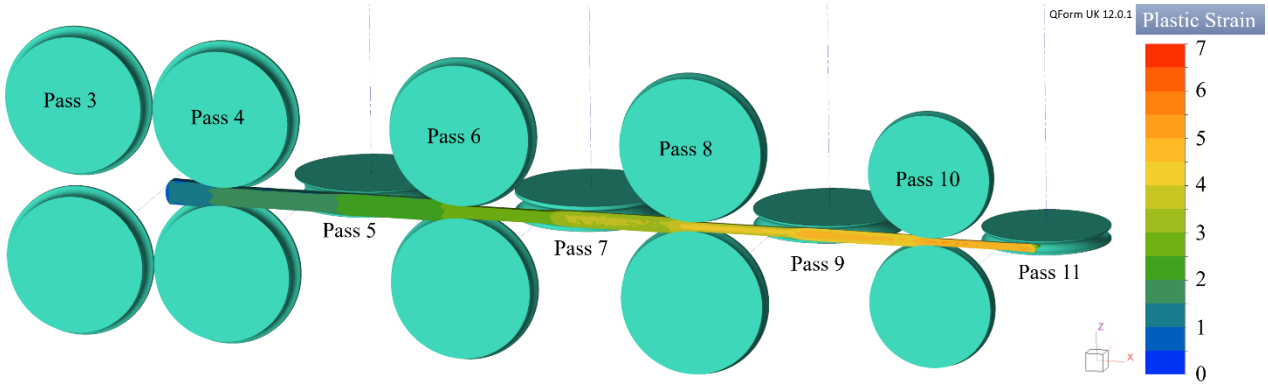


Fig. 2. Simulation of passes 3 to 11 of the rolling process in QForm UK® (longitudinal cross-section). Vertical rolls are used in the model to represent billet rotation between passes. Each stand is marked according to the corresponding pass number listed in Table 1. Passes 1 and 2 are simulated as a separate operation and are shown on Fig. 1b.

Challenges in measuring in-process data on a real mill. In an actual rolling mill, it is extremely difficult to obtain measurements of the material's state between stands. Mill operations cannot be halted mid-process to extract a sample, since the workpiece is at high temperature and moving at speed. As a result, plant engineers typically know only the input conditions (billet dimensions, temperature, etc.) and the final output properties (e.g., final dimensions, surface quality, mechanical properties after rolling). What happens to the microstructure or temperature in between passes is largely inferred rather than directly observed [7]. For example, one might like to know the austenite grain size after the third stand to calibrate a microstructure evolution model, but there is no practical way to stop the process and physically examine the grain structure, as the material must continue rolling to the end. These inherent experimental difficulties mean that purely empirical approaches cannot fully explain the evolution of microstructure and temperature during multi-pass rolling. We

have only snapshots before and after the rolling sequence, but not the full picture of what happens at each stage.

Because of this lack of intermediate data, numerical simulation becomes a crucial tool. By simulating the process, we can look at the state of the material between stands, for example, predicting temperature gradients, phase transformations, or grain size after each pass, the information that cannot be measured on the operating mill. Simulation allows us to adjust and optimise the rolling schedule.

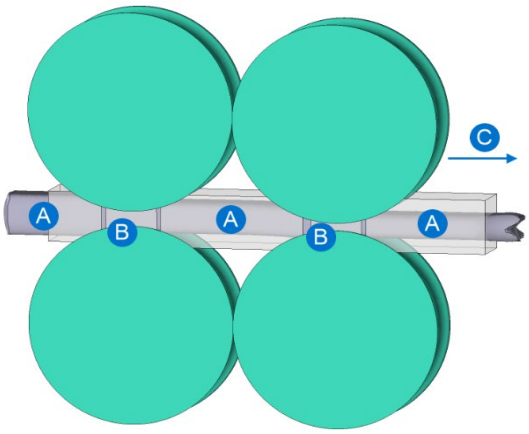


Fig. 3. Boundary conditions applied in the QForm UK® simulation of hot rolling: (A) extension boxes used for time-scaling to account for inter-stand distances; (B) water cooling; (C) rolling direction.

Accounting for real process time and cooling in the simulation. One important consideration in simulating multi-pass rolling is time scaling, which ensures that the thermal history in the model matches reality. In a real mill, the stands are relatively far apart, and it takes some time for the material to travel between them, while the total bar length increases significantly. Directly simulating an entire 50–100 m long bar moving through a long rolling mill is computationally expensive. Instead of a straightforward but computationally inefficient approach, a more specialised method based on so-called "extension boxes" was used in the simulation (Fig. 3) [8]. An extension box is essentially a segment in the model that introduces a delay or extra length of material to simulate the distance between mill stands. When the workpiece enters an extension box region, no further plastic deformation occurs, but the simulation continues to solve heat transfer for a specified duration, allowing the material to cool similarly as it travels the real large distance to the next stand. In other words, we scale the simulation time to match the real process time for each interval. This ensures that phenomena such as inter-pass cooling and any metallurgical transformations (e.g., static recrystallisation or phase changes during transportation between stands) are captured.

Methodology – Thermo-Mechanical Treatment Simulator

Description and simulation. The Thermo-Mechanical Treatment Simulator (TMTS) by Servotest Testing Systems Ltd is a sophisticated laboratory system capable of replicating industrial metal forming processes, combining high-force hydraulic deformation with precise heating (furnaces, induction) and rapid quenching to study how heat and mechanical stress affect metal properties, useful for research and development involving advanced materials like steels and alloys. It uses servo-controlled manipulators to move specimens between heating, deforming, and cooling stages, simulating complex industrial processes and has thus been widely used to simulate hot-rolling [9].

When combined with FE modelling of the rolling process, TMTS can be used to replicate the thermomechanical histories and conditions in the investigated material. To achieve these deformation histories (i.e., temperature, plastic strain, strain rate, mean stress, triaxiality, etc.), their graphs can be exported from rolling simulations, and then a TMTS experiment can be carefully designed to match these histories (Fig. 4).

The TMTS machine is well-suited for reproducing many aspects of complex multi-step industrial processes. In the context of the 11-step rolling chain considered in this study (Table 1, Fig. 2),

deformation levels beyond the sixth pass would result in extremely high strains exceeding 2.0, which, under the TMTS's uniaxial loading regime, would produce specimens thinner than 1 millimetre. To ensure realistic and reliable experimental conditions, the investigation therefore focused on the first six rolling steps. Importantly, the thermomechanical conditions in these initial stages were readily and accurately replicated in the TMTS FE simulation, enabling high-quality data generation for AI model development.

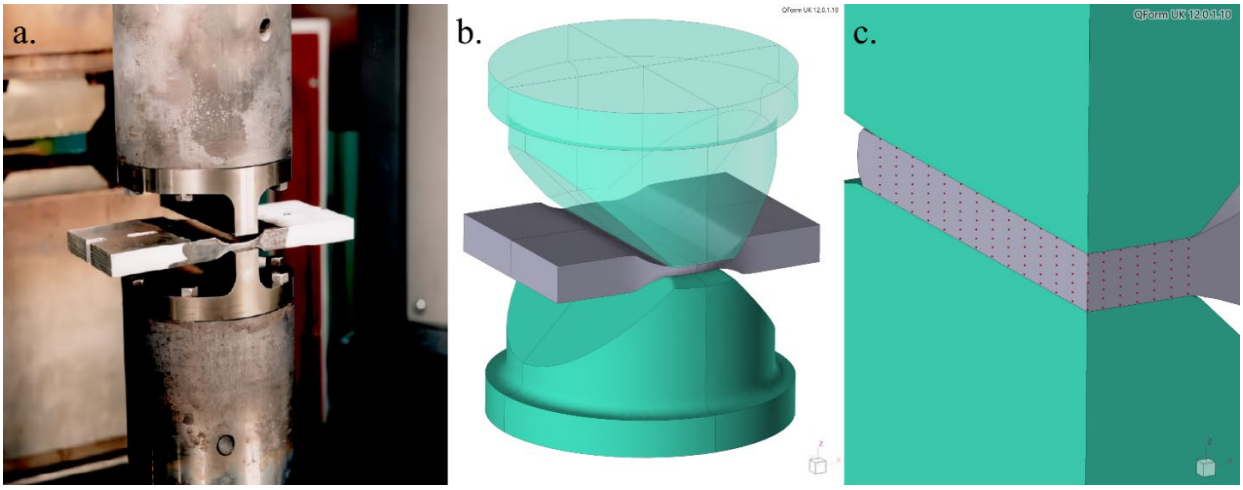


Fig. 4. TMTS experimental setup and simulation model: (a) photo of TMTS machine tools with kind permission of Servotest Testing Systems Ltd; (b) corresponding simulation model; (c) example of tracing point placement over the workpiece's cross-section at the end of one of the deformation operations.

Methodology – AI Microstructure Evolution Modelling

Synthetic data used in trial. As the final goal of this investigation is to construct an AI model capable of predicting complex microstructural evolution during multi-step industrial processes, and the data is synthetic, a target model for AI prediction must first be chosen. For this, a standard version of the Johnson - Mehl - Avrami - Kolmogorov (JMAK) [10] model included in QForm UK® software was chosen [11]. As this data is synthetic, custom coefficients for the model could be chosen. Thus, coefficients were tailored so that all types of recrystallisation (Dynamic (DRX), Meta-Dynamic (MRX) and Static (SRX)) would play a significant role in the process (Table 2, Fig. 5). However, during AI model training, only the total recrystallisation (RX) fraction was used as the target output. This reflects experimentally accessible data: total RX can be measured across a specimen's cross-section using optical or electron microscopy, whereas individual mechanisms and their interactions are far more difficult to quantify.

Table 2. Model parameters for each type of recrystallisation mechanism from QForm UK® microstructure evolution module [11].

Critical strain		DRX		SRX		MRX	
Ac	0.00396015	βd	0.693	βs	0.693	βm	0.693
Mc	0	Ad	8e-11	As	4	Am	3.16
Lc	0.1238	Md	0.2	Ms	0	Mm	0
Qc	49520	Nd	0	Ns	-0.75	Nm	-0.75
Cc	0	Ld	0.1	Ls	0.1	Lm	0.1
		Qd	270000	Qs	45000	Qm	45000
		Cd	0	Cs	0	Cm	0
		Kd	1	Ks	1	Km	1

Methodologically, predicting multiple JMAK mechanisms is also considerably more challenging for a single AI model, making total RX a practical and robust target. At the same time, this strategy tests whether the model can implicitly distinguish and reproduce qualitatively different

recrystallisation behaviours using only thermomechanical loading histories and the resulting total RX evolution. No explicit information about the underlying mechanisms is provided, so any successful differentiation emerges purely from the learned correlations.

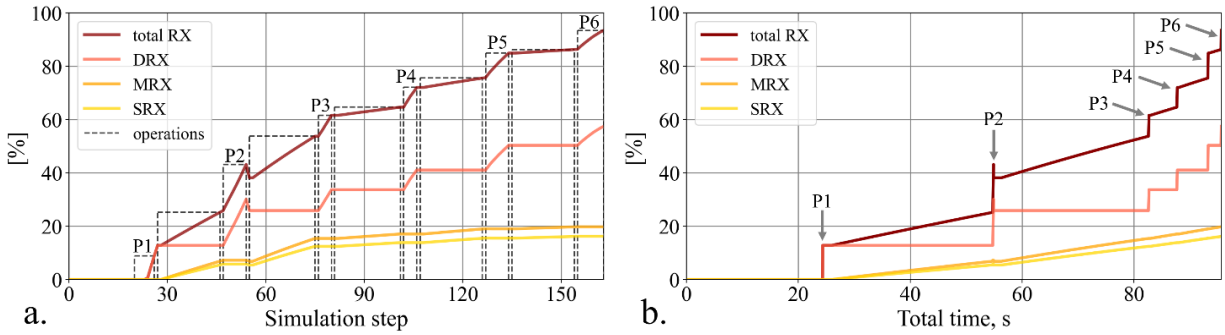


Fig. 5. JMAK model values traced from a point in the centre of the specimen over full TMTS simulation: (a) plotted over simulation steps; (b) plotted over time. P*i* – denotes the *i*-th deformation operation, replicating the *i*-th rolling pass (Table 1), with heat-treatment operations in between.

AI model inputs. As the chosen AI architecture is an RNN, it takes as input complete thermomechanical histories in order to predict RX evolution along those trajectories. To be more specific the following values are passed to the model at each step directly from the FE simulation: time step [s], temperature [°C], accumulated plastic strain, strain-rate [1/s], effective stress [MPa]; and also the following histories are calculated on top of these values and also passed to the model: plastic strain increment, effective stress increment, plastic work, plastic work increment and the Zener–Hollomon parameter. Thus, the model takes 10 values as input at each time step. These values are also linearly normalised before use in the AI model. The specific set of input histories was chosen based on the author's previous microstructural modelling experience. More specific information on this choice and how these values are calculated can be found in [5].

Data preparation. Only the TMTS simulation is used to train the AI model. For this at the end of each operation two arrays of points are mapped over the middle cross-sections of the specimens working area: a 7 by 7 array in the XZ plane and a 14 by 7 array of points in the YZ plane (Fig. 4c). This is done for each of the 6 heat-treatment and 6 deformation operations for a total of 1680 training points. Each of these points' paths is tracked from the beginning of the simulation to where they were created. Then, full 10-value model histories listed above are exported, as well as final single total RX values, which serve as the target prediction values for the AI model during training.

This is repeated two more times for simulations with doubled and quadrupled simulation step lengths for a total of 5040 training pairs of thermomechanical loading histories and corresponding total RX values. Histories from simulations with doubled and quadrupled simulation step lengths should be included in the dataset, as the AI model doesn't have the same considerations built into its architecture as a standard incremental analytical model, given that its behaviour is primarily data-driven. Expanding the dataset in this way will help stabilise the model's behaviour for histories with different step lengths, which is a necessary quality for it to be usable in conjunction with FE simulation. This data is also generally useful for expanding the AI training dataset and for verifying the input simulation. As expected, RX values are identical at the same points in simulations with different time steps.

AI model and training description. As mentioned earlier, the AI model architecture consists of an RNN model, which takes as input 10 time series of arbitrary length. The recurrent cell chosen for the model is an LSTM cell [4] with a custom physics-based augmentation. The cell maintains hidden state vectors for long-term (C) and short-term (H) memory of size 10, and is augmented such that the first value in C is strictly non-decreasing and is bounded between 0 and 1, ensuring it respects RX physical constraints, as this value is used as the model's scalar output.

The model was trained for 10000 epochs with the Adam optimiser, minimising the mean square error between RX values and the model's output predictions at the chosen points. 90% of the dataset was used for training, with the remaining 10% reserved for validation.

This architecture was previously trained on experimental data and successfully used to predict recrystallisation during single-step hot forging of Inconel 718 [5]; however, multi-step processes remain particularly challenging due to the lack of an experimental methodology to address them, which this paper aims to address.

Results

After the model was trained, two methods were employed to test its predictive capabilities, both in TMTS and rolling simulations:

1) Thermomechanical loading histories were exported from FE simulations at key points and were used as model input for direct comparisons.
2) The trained model was implemented as a Lua user subroutine for QForm UK®, allowing it to be tested directly in FE simulation.

AI predictions in TMTS simulation. Both training and validation accuracies during the calibration process exceeded 99%. When tested in the TMTS FE simulation, JMAK RX fields match AI-predicted RX fields nearly perfectly (Fig. 6) across the entire specimen volume and all simulation steps.

Traced data plots of JMAK and AI predicted RX values in several key points show that the AI model is able to predict RX evolution properly in completely different loading regimes (Fig. 6c). These specific points are not from the set of all training points (Fig. 4c), however they do come from the same overall domain and have very similar loading histories to some of the points used in training.

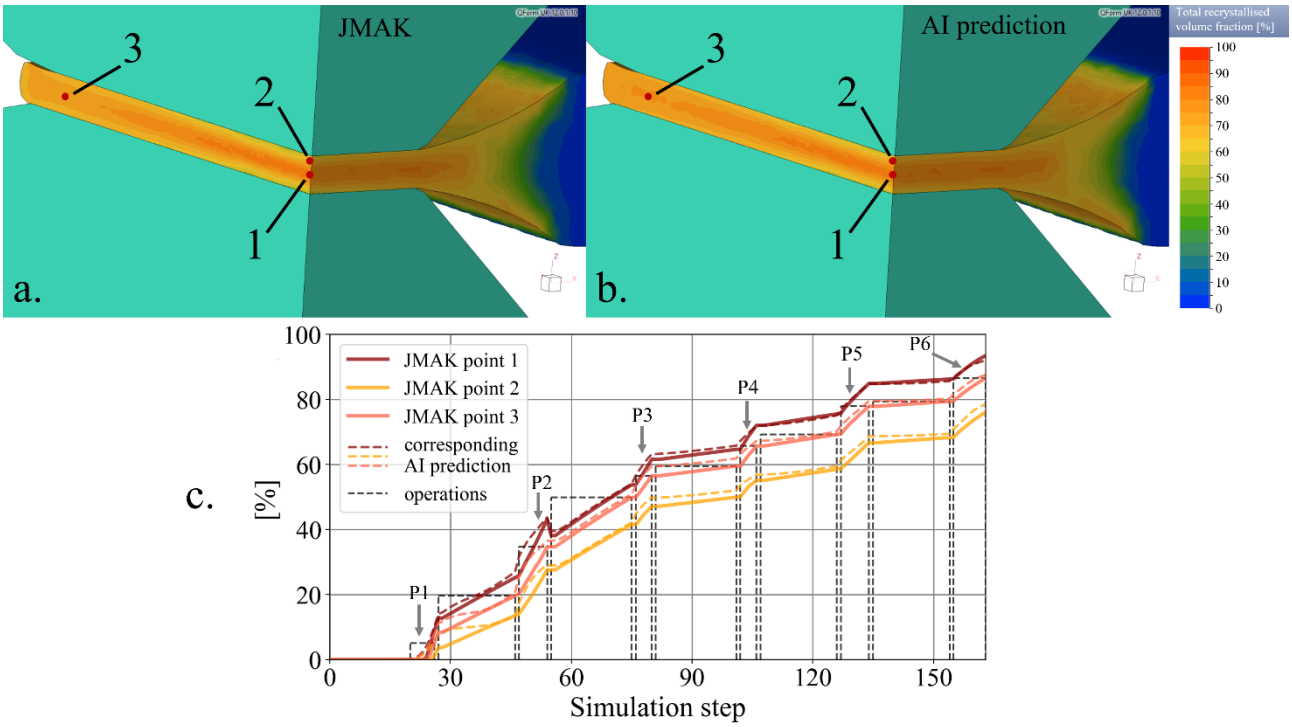


Fig. 6. Comparison of initial JMAK model and AI predictions in TMTS simulation: (a) JMAK RX field and point locations; (b) AI predicted RX field; (c) JMAK and AI predicted RX values plotted over full simulation duration for points highlighted in (a, b). P*i* – denotes the *i*-th deformation operation, replicating the *i*-th rolling pass (Table 1), with heat-treatment operations in between deformations.

AI predictions in the initial rolling process simulation. A qualitative analysis of the results shows that the AI model has indeed identified the different types of RX models and can distinguish between them solely based on thermomechanical loading conditions, even within a highly complex FE simulation of a multi-step hot-rolling industrial process.

Quantitatively, the results are interesting. As shown in (Fig. 7), in some points (1, 5, 7), prediction results are very accurate, with errors under 5% RX. However, other points (2, 3, 4, 6) exhibit errors ranging from 10 to 20% in the final RX prediction. In point where prediction errors are significant, most of the deviation accumulates at the first few rolling passes, with parallel JMAK and AI predicted RX curves and no more error accumulation at later stages.

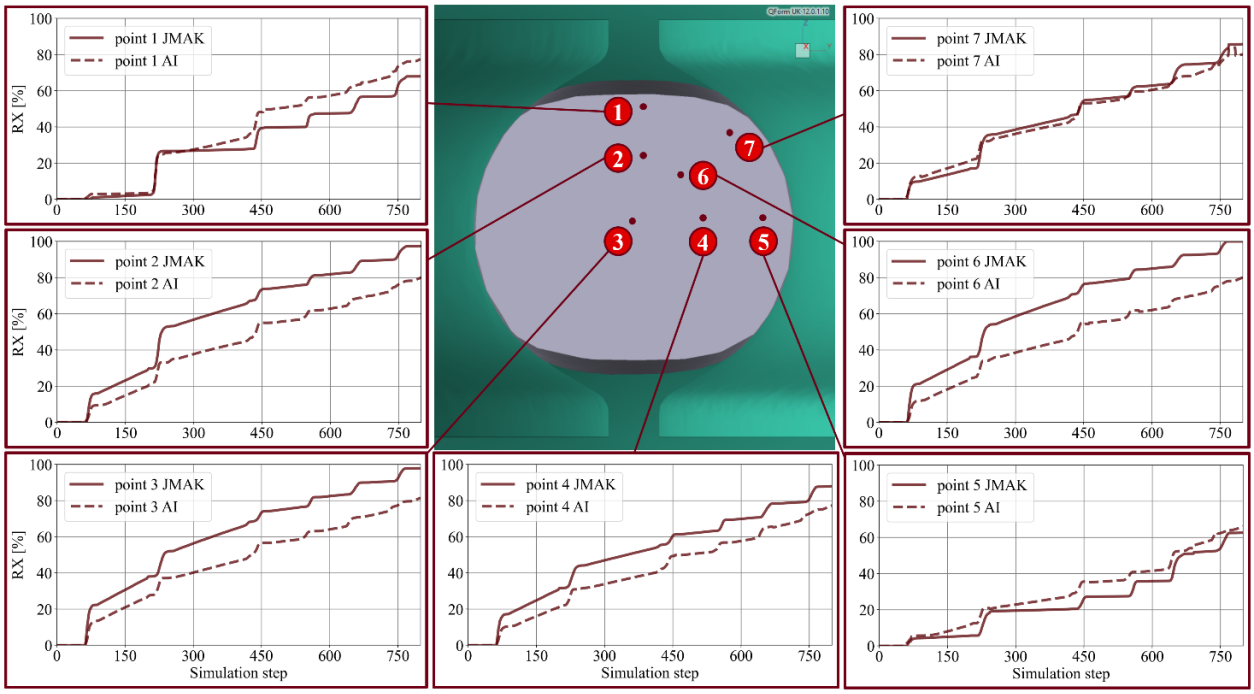


Fig. 7. Comparison of the initial JMAK model and AI predictions in the original rolling simulation for multiple key points over the billet's cross-section.

Discussion

This result is somewhat expected, as the TMTS simulation used for training was constructed solely from a single traced loading history from the rolling simulation, whereas different histories can be observed at different points within the billet. Indeed, the points where prediction is most accurate (Fig. 7, points 1, 5, 7) are closer to the outer edge, whereas the other points are closer to the billet's centre. This distinction is more obvious when analysing loading histories at these points (Fig. 8). The JMAK model, used for synthetic target data, is governed by three main parameters: the temperature, plastic strain, and strain-rate. The plastic strain and strain-rate histories are very close regardless of point location over the billet's cross-section (Fig. 8c,d). Temperature, however, varies significantly: points closer to the edge experience much more cooling (Fig. 8a,b). This difference is most significant during the first few rolling passes, consistent with the areas of error accumulation observed in the results for points closer to the billet centre.

The TMTS simulation was initially constructed based on a single loading history; as such, the training points mapped over its cross-section (Fig. 4c) exhibit different but similar loading histories, representative of the variety of loading regimes found in the rolling process, in terms of plastic strain and strain rate, but not so in Temperature. Moreover, temperature deviation during the TMTS simulation was generally much lower than in the rolling simulation, with a nearly uniform temperature field throughout the workpiece volume. From this, it can be inferred that the AI model had very little information from which to determine the significance of temperature for RX formation in the JMAK model, which, in reality, plays a large role. This significantly narrows the range of applicability of the trained model and highlights the importance of conducting multiple tests and or simulations with varied loading regimes to diversify the training data set. Ideally, when using the TMTS machine or similar equipment to replicate a multi-stage industrial process, histories from different parts of the billet should be considered for replication, along with some random variation in those histories, reflecting the possible instability in reproducing real-life industrial conditions.

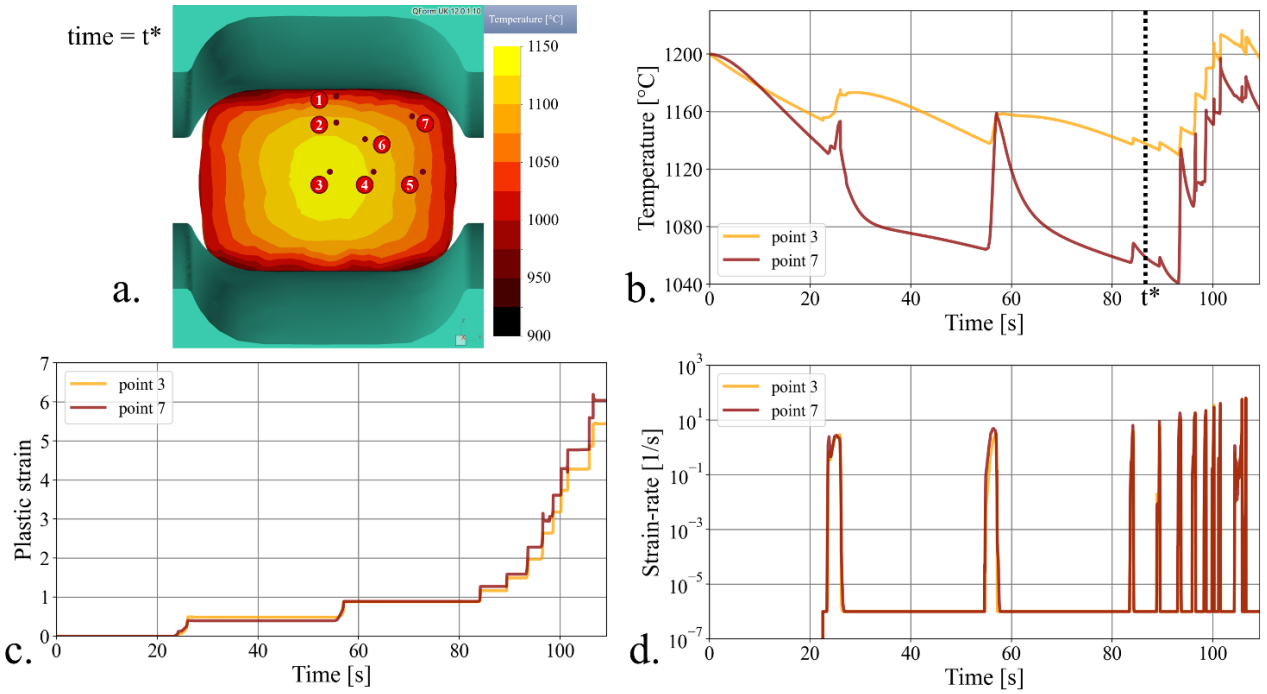


Fig. 8. (a) Temperature field over billet cross-section at time t* between rolling pass 3 and 4 (Table 1); curves over full 11-pass rolling simulation, characteristic for inside (3) and outside (7) points: (b) Temperature; (c) Plastic strain; (d) Strain rate.

It is also of note that the JMAK model, used in this work as a substitute for experimental microstructural data, isn't able to faithfully represent all the mentioned mechanisms and cannot be truly predictive in a general sense for microstructure characteristics during complex hot metal forming processes. This has been shown by various independent benchmarking studies [1, 2, 12]. Real experimental data could vary significantly and could possibly be more challenging for the AI model to reproduce. However, the AI model is a much more robust and generalised tool and isn't actually tied to the JMAK model in any way. The AI model's ability to reproduce JMAK model results in complex loading regimes is only a reflection of its robust data-driven foundation. The model's applicability to experimental microstructural data has already been shown in single stage forging processes [5]. It's applicability to practical multi-stage processes as well as to a wider range of predicted values, such as grain size, will be thoroughly tested in further works.

Conclusion

This paper presents a novel AI-based approach to developing microstructural models for multi-stage hot deformation processes. The core challenge, acquiring intermediate experimental data for model calibration in industrial settings, is addressed by integrating FE simulation in QForm UK®, physical laboratory testing using the TMTS machine, and a physics-informed artificial intelligence model.

The methodology was demonstrated through a case study of 11-pass hot rolling of 41Cr4 steel. A FE simulation of the process provided complete thermo-mechanical loading histories. Such histories informed a targeted Thermo-Mechanical Treatment Simulation (TMTS) test, also modelled in FE software, which replicated a critical stage of the rolling sequence to generate intermediate microstructural data. A JMAK model, incorporating DRX, SRX, and MRX mechanisms with specifically tailored coefficients, was used to synthesise a comprehensive microstructure evolution dataset. A recurrent neural network with a custom physics-augmented LSTM cell was then trained on this dataset to directly predict the total recrystallised fraction from the thermomechanical input histories.

The results demonstrate that the TMTS machine is a viable tool for reproducing thermomechanical loading conditions of multi-step hot rolling under laboratory conditions, although the use of uniaxial

compression limits the maximum achievable strain and restricts accurate replication of later rolling passes with high deformation. Additional experiments may also be required to capture the strong spatial non-uniformity of industrial billets, particularly due to temperature gradients and surface cooling. Despite these constraints, the combination of TMTS physical simulation and FE modelling proved highly effective for generating comprehensive thermomechanical and microstructural datasets, enabling a robust data-driven machine-learning approach to microstructure evolution modelling. The trained AI model was successfully implemented as a Lua subroutine in QForm UK® and validated against both TMTS and rolling simulations, confirming its accuracy and robustness. The main contribution of this work is a practical integrated framework that unifies FE modelling, physical simulation, and AI for modelling complex multi-step industrial processes where conventional experimental approaches are impractical, while emphasising the critical role of strategic experiment design in bridging laboratory and industrial conditions.

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