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The prospects of implementation of artificial intelligence for modelling of microstructural parameters in metal forming processes

TRETYAKOV Denis[1,3,a], BYLYA Olga[2,b], SHITIKOV Andrei[4,c], GARTVIG Artur[1,d], STEBUNOV Sergey[1,e], BIBA Nikolay[4,f*]

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

[2]National Manufacturing Research Centre, University of Strathclyde, 3 Netherton Sq, Paisley, Renfrew PA3 2EF

[3]Moscow State University, Lomonosovskiy Prospekt, Moscow, Russia

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

[a]tretyakov.denis.a@gmail.com, [b]olga.bylya@strath.ac.uk, [c]a.a.sh.ggml@gmail.com, [d]gartvig@qform3d.com,[e]serg@qform3d.com, [f]nick@qform3d.com

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Abstract. The primary trend in modern metal forming can be characterised by the increase in the complexity of the technological processes and higher demand for the quality of the products. This naturally raises the requirements for the quality of modelling prediction of various aspects of metal forming process, such as tool wear, metal flow, fracture and defects formation, microstructure evolution and mechanical properties. However, various independent benchmarking studies [1] have shown that modelling predictions can be wrong even for well-calibrated models, and all the efforts with more detailed and metrologically better experiments didn't lead to any significant leap in the prediction quality. As an attempt to implement some alternative approach, this paper investigates the applicability of an Artificial Intelligence (AI) approach, in particular Deep Learning models. The example of a recurrent neural network model predicting recrystallisation during hot forging of Inconel 718 is presented. The model considers the entire thermo-mechanical history at every point and is trained and blind-tested using actual experimental data.

Introduction

The author's experience shows that there exists a certain scepticism about AI-based models among people involved in microstructural modelling in the industrial and scientific fields. It is often said that analytical models describing various phenomena involved in metal forming reflect the "physics" of the process and can, therefore, be trusted, while AI models are a sort of "black box" somehow trained to guess few correct answers and can't be reliable. Both parts of this assumption are not true. Almost all classical phenomenological models are the curve-fitting of experimental data accompanied by logical interpretations of the observed trends and dependencies. This nature is the origin of the major limitations of such models, i.e. their mathematical structure and long, costly and complicated calibration, i.e. the process of finding actual model parameters [2].

Taking recrystallisation as an example and assuming that it depends on only three major process parameters: strain, strain-rate and temperature, the relation for recrystallisation should be written as a differential to reflect history dependence, i.e. $dR/dt=f(T, \varepsilon, \dot{\varepsilon})$. For calibration of this model, we can change only one parameter at a time; others should be fixed, though it can be technically difficult. Thus, to get data for just three temperatures, strains and strain-rates, a minimum of 9 experiments are needed and a total of 36 for four strain values [3-5]. As a result, identification of the model parameters, in reality, is always based on a very limited number of points (which limits the mathematical complexity of the model), with limited strain value (generally not more than 0.7),

and an assumption that the reactions on individual parameters are additive and transients in parameter changes are negligible. This forces the model to use plenty of extrapolations when utilised in real industrial processes and often causes poor results.

Returning to the second part of the first statement regarding AI models. As it will be shown in this paper, the principle of their operation is not much different from phenomenological models. The recurrent cell used in the modelling of recrystallisation is analogous to the above-mentioned R, with a few additional state variables dR/dt=f(T, ε, έ, R, h1, h2, h3, …), having a different numerical representation and a bigger number of model parameters. This substitute is based on the universal approximation theorem established by Cybenko [6], which states that a neural network with one hidden layer, a finite number of neurons and a sigmoid activation function can approximate any continuous n-dimensional function with any set precision.

The second peculiarity of the AI models is the technique of their calibration or "training". Traditional analytical models could not use data directly from industrial forging processes because of complicated thermo-mechanical histories, as manual curve-fitting needs to change one parameter at a time. In contrast, machine learning utilises finding model parameters based on recognising patterns from data. In this case, the complexity of the data is compensated for by its amount.

Summarising everything mentioned above, AI-based models have quite a similar phenomenological nature but with a more flexible mathematical structure and advanced calibration techniques. Their implementation in process modelling can simplify the process of tuning models for metal forging industries. Industrial forging data can be used directly instead of "special" uniaxial lab tests. This will also improve the prediction quality because the model will work in the regime of interpolation. An example of one such model is presented in this paper.

Methodology

Forging trials. The quality of model calibration is always extremely dependent on the quality of the experimental data. For analytical models, it is critical to keep only a single process parameter changing and others fixed, limiting specimen geometry and loading parameters. For AI models, these restrictions are unnecessary, and forged parts of different geometry can be used. In this investigation, the relatively simple geometry of Double Truncated Cones (DTC) was used for model calibration, and more complicated profiled disk geometry for blind validation (Fig.1a). Forging trials were performed on an industrial 21 MN screw press (Fig.1b) at the temperatures 970°C and 1080°C. During the experiment, the ram velocity and energy were recorded on the press and temperature distribution was measured with three thermocouples embedded in the specimen (Fig.1c). All this data was used for the validation of FE simulations of the forging processes performed in the commercial metal forming simulation software QForm UK®. After forging, specimens were quenched in water, cut and analysed under optical and electron microscopes. The obtained distribution of the percentage of recrystallisation over the specimen's cross-section is shown in Fig.1d. More information on these experiments and experimental results can be found in the following papers [7, 8].

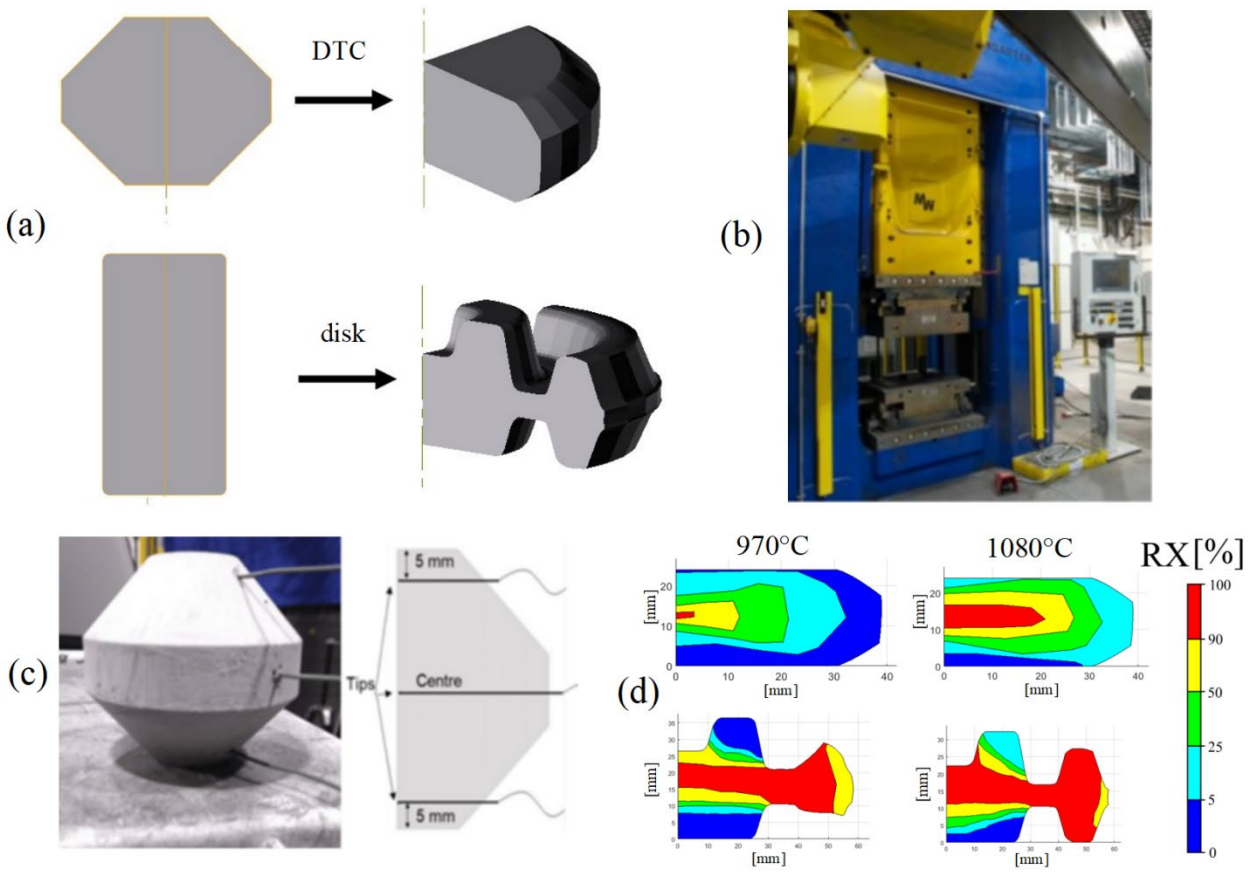

Figure 1. Forging trials: a) geometry of the parts; b) screw press; c) location of thermocouples; d) experimental distribution of recrystallisation.

Extracting Data from FE models. It's crucial that the FE models of these processes are calibrated correctly before any further work can be done, as the data acquired from these models will later be used for training the microstructural models in question. This is why data such as energy and movement of the press as well as specimen temperature over time at multiple points is absolutely necessary to validate the model [7]. More detailed information on the constitutive model and FE simulations used in this paper as well as the methods used to calibrate and validate them can be found in the following papers [7, 8]. After the model is validated, a large distribution of points is chosen over the specimen. Using modern FE modelling software such as QForm UK® we can extract full thermo-mechanical histories over the course of the simulation for each of the chosen points $[T(t), \varepsilon(t), \dot{\varepsilon}(t), \dots]$.

Unlike in traditional lab experiments performed on small specimens in a presumed homogeneous state where these values are constant over the whole specimen and in time, we used more complicated industrial forgings where these histories are vastly different at different points in the specimen and are far from constant in time (Fig 2.), this can also be seen from analysing the drastically different temperature profiles from the three thermocouples [1]. This fact, combined with the new opportunity to extract complete thermo-mechanical histories from different points of a specimen, allows us to gather an unprecedented amount of data from just a few industrial forgings. Having analysed the cross-section of our specimens at the chosen points, we can now map the thermo-mechanical histories to their corresponding resulting microstructural parameters such as percentage of recrystallisation, grain size and others. For simplicity, only the percentage of recrystallisation was considered in this study. An additional bonus of this large body of data is

that it lends itself very well to a machine learning approach that, despite its benefits mentioned earlier, requires a lot of training data to be implemented successfully.

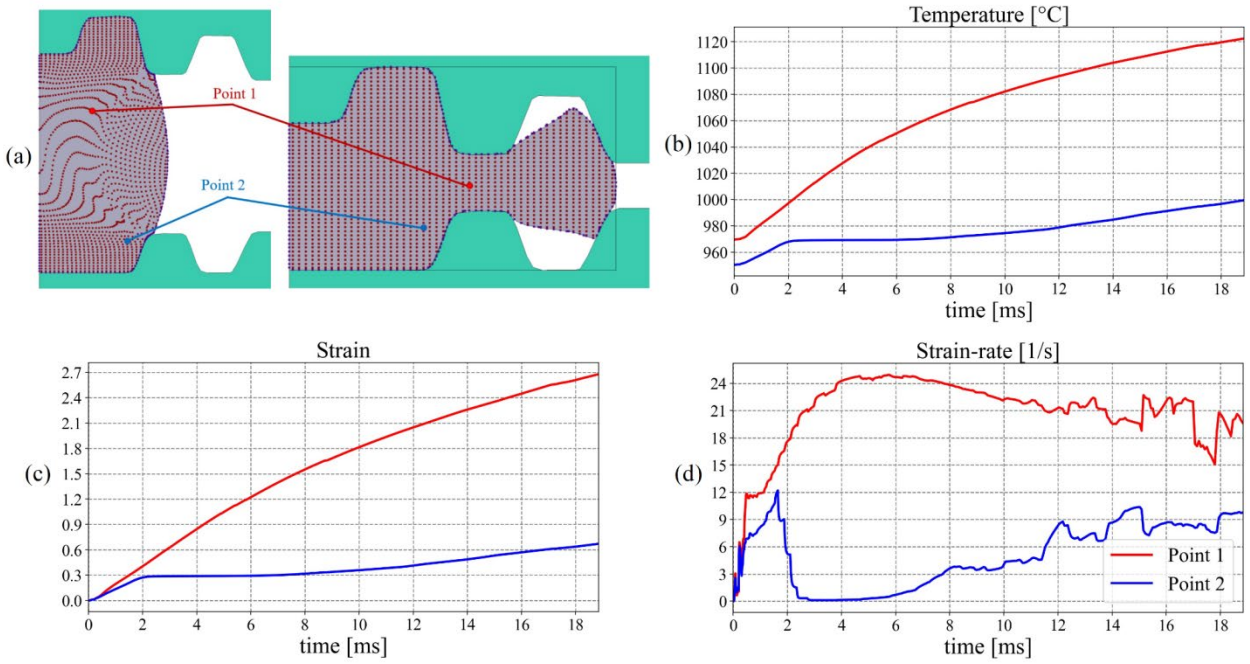

Figure 2. Example of numerical data: thermo-mechanical histories at two different points of the specimen: a) locations of two different points in two configurations of the deformed part; b) temperature over time at chosen points; c) strain over time at chosen points; d) strain-rate over time at chosen points.

AI model. The model consists of a recurrent neural network with a long short-term memory (LSTM) cell [9] with a hidden state vector of size 10 as the recurrent cell. The LSTM cell was modified so that one of the values of the hidden state vector would start at 0, wouldn't decline with each time step and wouldn't exceed 1; this value was used as the output of the model.

The model includes a total of 840 trainable parameters. As for the training data, exactly two forgings were used to calibrate the model: DTC at 970°C and 1080°C. For both of these forgings four FE simulations with different time step lengths were made in QForm UK®. This was necessary to ensure consistent behaviour of the trained model when applied to the same FE simulation with differing time steps, as this isn't inherently part of the models' architecture. From each of these eight simulations, around 1500 points in a uniform grid in finish configuration were chosen, as shown in (Fig 2a) for a total of 12000 training points. Thermo-mechanical histories used for training the model from each of these points consisted of the following 10 values at each time step that form the vector x:

$$x = [dt, T, \varepsilon, \dot{\varepsilon}, \sigma, d\varepsilon, d\sigma, dW, W, ZH]$$
$$dt - Time\ Step\ [s]$$
$$T - Temperature\ [°C]$$
$$\varepsilon - Accumulated\ Plastic\ Strain$$
$$\dot{\varepsilon} - Strain - Rate\ [1/s]$$
$$\sigma - Effective\ Stress\ [MPa]$$
$$d\varepsilon = \varepsilon_i - \varepsilon_{i-1}$$
$$d\sigma = \sigma_i - \sigma_{i-1}$$

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$$dW = \sigma \cdot d\varepsilon$$
$$W = W_{i-1} + dW$$
$$ZH = \dot{\varepsilon} \cdot exp\left(\frac{Q}{R \cdot T_{abs}}\right)$$

where $Q - Activation\ Energy\ [J \cdot mol^{-1}]$, $R - Gas\ Constant\ [J \cdot K^{-1} \cdot mol^{-1}]$, $T_{abs} - Temperature\ [K], i - index\ of\ time\ step.$

The choice of process parameters included in x was based on preliminary data analysis and previous microstructural modelling experience.

The training data was normalised and split into 80 batches. The model was trained for 500 epochs with an ADAM optimiser, minimising the mean square error between experimental recrystallisation percentage values and the model's predictions at the chosen points.

A benefit of using such architecture is that the trained recurrent cell can be implemented in metal forming simulation software and run during FE simulations using data from the simulation at each step as input and feeding microstructural data back into the material model if needed. After the model was trained, it was implemented as a Lua user subroutine in QForm UK® for further testing and analysis. The model was blind tested on simulations of the profiled disk forgings.

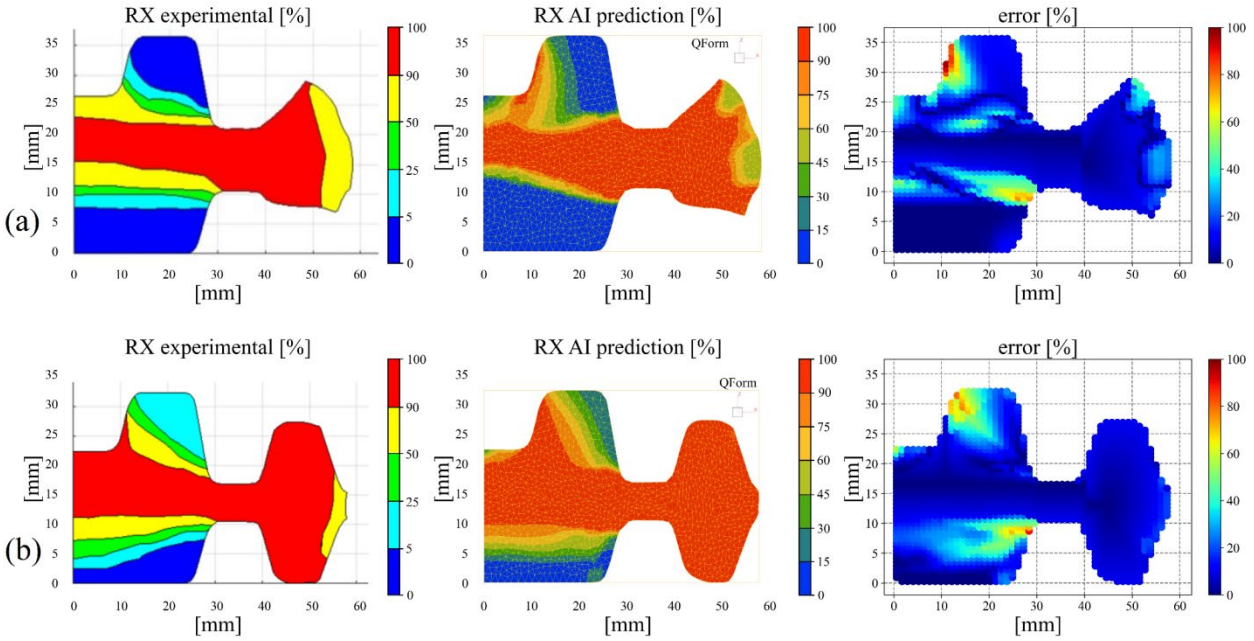

Figure 3. The results of the blind test of the proposed AI-based model: a) disk forged at 970°C; b) disk forged at 1080°C.

Results

A comparison of results from the FE simulations of the forging processes with the AI-based model used as a user subroutine against experimental data is shown in Fig. 3. Analysing obtained results, a few important points should be emphasised:

1. Despite the fact that the disks trials were used as a completely blind test for the model, the acquired results are physically consistent, and the field of the percentage of recrystallisation is smooth and continuous over the specimen and over time. Traditional analytical models are mathematical formulae describing the relations between different process parameters. They are generally expressed as smooth, continuous functions differentiable with respect to time and coordinates. On the other hand, such smoothness and continuity are not a generic property of an AI-based model's architecture. Thus, the continuity observed in the blind tests shows that the model succeeded in identifying some process features from the provided data during training.

2. Quantitative results of the blind tests are surprisingly good. The profiled disks have more complicated geometries, and they were obtained in a "closed die" forging process, which leads to more complex process histories than the ones used to train the model, and this will be discussed in more detail later in the paper. However, out of 1500 traced points, the error in prediction was more than 30% only for 250 points in the 970°C trial and about 300 points for the 1080°C trial (Fig.3).

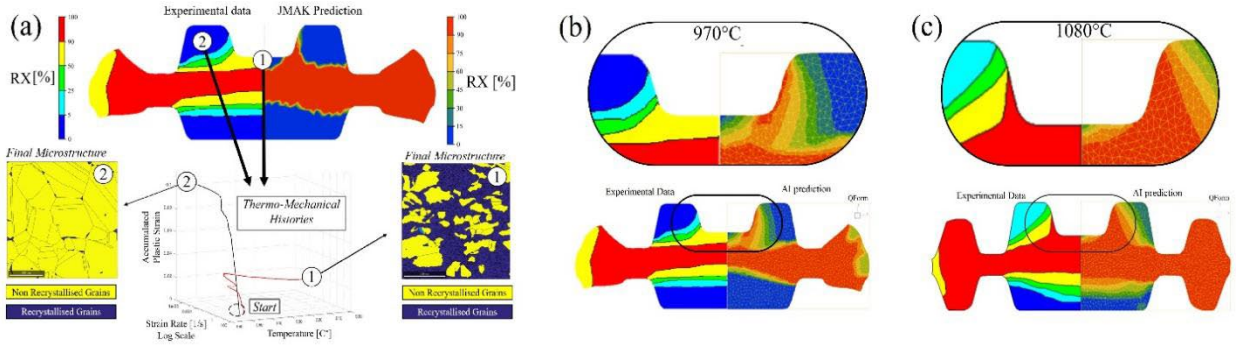

Figure 4. Peculiarities of the AI-based model: a) some puzzling microstructural results; b) comparison of the AI-based model prediction with the experimental results in the questionable zone for disk at 970°C; c) the same for disk at 1080°C.

3. Microstructural analysis of the profiled disks of the given geometry forged on a screw press yields some puzzling peculiarities of this process [2,7], which, in principle, can't be described by any JMAK-type model. As shown in Fig. 4a, at the centre of the disk, at the point of first contact with the upper die there is a zone marked as "1", which, according to modelling and common sense, is characterised by very low strains as material there doesn't flow anywhere and relatively low temperatures due to contact with the 350°C die. However, this zone shows a very pronounced high level of recrystallisation, and this result is consistently reproducible. For comparison, in a zone marked as "2" with higher strains and temperatures, only a few sparse recrystallisation nuclei were observed. It was unexpected to see that the utilisation of an AI-based model helped predict recrystallisation in zone "1" in both blind tests (Fig. 4c). Most likely, this means that in the process of training the AI-based model was able to isolate some hidden correlations in the data, reflecting not very evident mechanical or microstructural mechanisms, which is a natural for deep learning algorithms.

Despite having trained the AI-based model on data from only two industrial forgings, the model outputs competitive results when compared to traditional JMAK based models. Fig. 5 shows the results of AI prediction against one of the most popular traditional JMAK models [10] used as default in multiple commercial metal forming simulation software programs, e.g. QForm UK® [11] and DEFORM® [12]. It can be observed that the AI model demonstrates a more correct qualitative distribution of recrystallisation levels. Comparing the figures of total recrystallisation level, it can be observed that the AI model has the capability to better describe intermediate zones between non-recrystallised and fully recrystallised zones (which is typically a weak point of all JMAK-type models). Quantitatively, the AI prediction is also better, however, this comparison is not completely fair as the AI model was calibrated for the same material as the one used in experiments with the profiled disks, while in the case of the JMAK model, standard default coefficients for Inconel 718 were used.

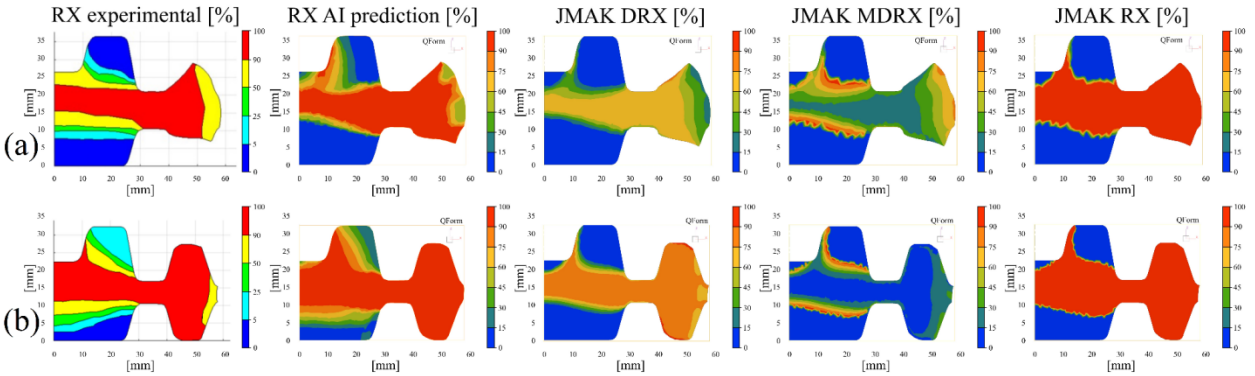

Figure 5. Comparison of the predictions of AI-based model and standard JMAK model for the "blind" tests - disks forged at the screw press at: a) 970°C and b) 1080°C.

Discussion

When it comes to implementing the described methodology and model in practice for modelling microstructure evolution in commercial forging processes, there are a few clear advantages and challenges compared to the methodology and models currently in use that we would like to discuss.

The potential predictive capabilities of an AI-based model, such as the one showcased in this paper, are far superior to a traditional analytical model, since the model itself has a much higher predictive capacity and can predict unknown dependencies found in the data without the need to describe them analytically. This was clearly shown with the "unexpected" prediction of recrystallisation shown in Fig. 4. It obviously could be argued that such results are nothing more than luck; meanwhile, only a large amount of further testing and data analysis with various other forgings can give a definitive answer regarding the robustness of the model. However, in our opinion, this is not random luck for the following reasons. Standard JMAK models use only three process parameters (temperature, strain and strain rate), assuming that the influence of other process parameters is negligible even though it was not proven by any investigation. As described in section 2.3., the model presented in this paper uses 10 process parameters, providing the artificial neural network the freedom to "decide" whether these parameters are essential for correct prediction of the results or whether they should be ignored. This may, for example, be important in the description of various transient, unsterilised processes where the role of gradients of the process parameters is not very clear but whose influence could have been picked up by the model during the training process.

Another example of a higher predictive capability can be seen in the comparison with the JMAK model (Fig.5). Screw press forging is a fast process where the total deformation takes just a few seconds. The time of the process is not sufficient for the material to absorb all the strain energy provided to it, and as such, the Dynamic Recrystallisation (DRX) initiated during the forging actively continues as Meta-Dynamic (MDRX) or Post-Dynamic Recrystallisation (PDRX) in the few seconds after deformation [13]. This is why JMAK-type models traditionally consist of three main parts: DRX, MDRX and SRX, which is Static Recrystallisation, which generally occurs during reheating or heat treatment [10-12]. Each part contains 7-10 material parameters, which are expected to be found analytically from pure uniaxial tests. Unfortunately, in practice, it's almost impossible to separate Meta-Dynamic from Dynamic recrystallisation; as such, the MDRX part of JMAK-type models often suffers from poor calibration (which can be observed in Fig. 5). Machine learning algorithms may help with this for two reasons. Firstly, as most of the information about the underlying mechanical and microstructural processes is acquired by an AI-based model and reflected in its parameters from the data, there is no need to actively separate these processes in the underlying architecture as long as they are both sufficiently represent in the experiments used

for calibration. Secondly, the fixed mathematical structure of a traditional analytical model with only 20 parameters may simply be too "stiff" for successful optimisation.

Speaking about other prerequisites of higher predictive quality, it should be noted that the proposed methodology for data collection and calibration from industrial forgings results in the model generally working in an interpolation regime. Models based and calibrated on uniaxial lab tests, on the other hand, are often forced to be used in an extrapolation regime as they attempt to process data from actual industrial forging processes that are far more complicated.

Nevertheless, the existing challenges must also be addressed when discussing the potential advantages of AI-based models. The main advantage of traditional analytical models comes from the capability to analyse their behaviour, though practically, this isn't easy to do for complicated models. Analytical models can give wrong predictions in extrapolation, but the worst scenario can be accessed at least theoretically. This is not the case for deep learning models. As mentioned earlier, the quality of AI-based models significantly depends on how well they recognise important data patterns during training. Developing the methodology for guaranteed successful training is a serious challenge in AI research and is beyond the scope of this paper. However, some steps can be proposed to increase the chance of successful training.

The key prerequisite of successful training is appropriate data. As mentioned in the introduction, training of an AI-based model is similar to curve fitting and consistency and homogeneity of training data may be more important than the total amount of data.

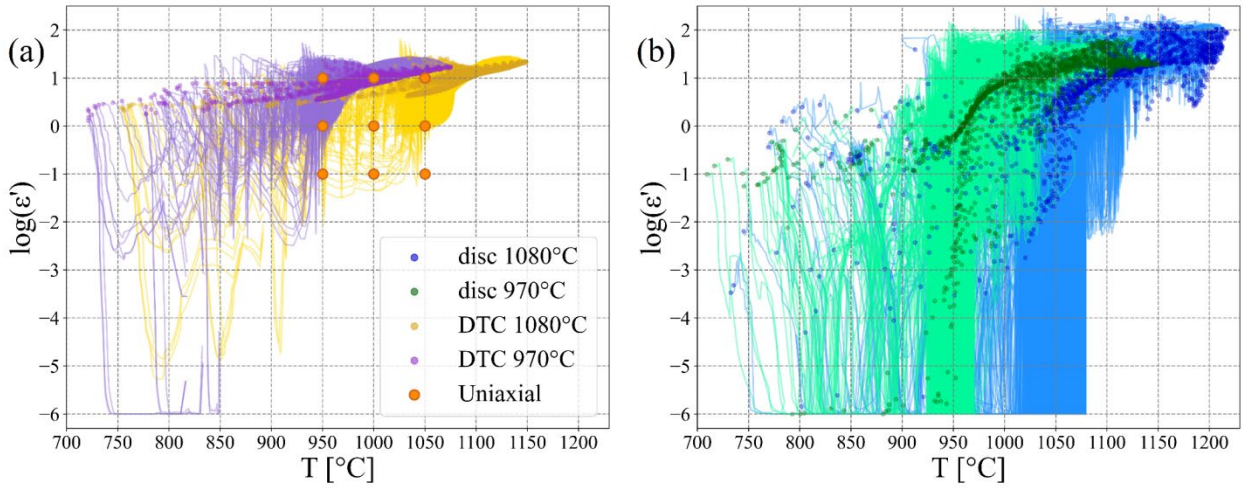

Figure 6. Projection onto the [Temperature, Strain-rate] plane of the data used: a) for training the AI model, b) for blind validation of the AI model. Orange dots represent process data from standard uniaxial lab tests generally used to calibrate traditional JMAK-type models.

Fig. 6a shows the data obtained from FE simulations of the two forgings of double truncated cones and the typical set of results that can be obtained from uniaxial lab tests. For each point of the DTCs, curved trajectories show thermo-mechanical histories traced at those points and a coloured circle – the final state. Uniaxial tests have constant temperature and constant strain rate, so they don't have a path in this space and are sufficiently denoted by a single point. The first thing to note in this figure is how far-reaching the data from the forging trials is compared to uniaxial tests. One single forging trial can provide hundreds of trajectories. It can also be observed that there can be vastly different histories resulting in the same or similar final states (the same can be said about points with similar experimental final recrystallisation values).

In the example showcased in this paper around 3000 trajectories were taken from just two forging trials and were successfully used to train 840 parameters. Is this dataset sufficient? Is the

quality of this dataset sufficient? What additional forging trials can improve model training? The answers to these questions are not evident. But in the first approximation, it can be concluded that good results in blind prediction show that an AI-based model was able to recognise important patterns that previously were not recognisable with a traditional approach. However, Fig. 6b shows that a significant amount of thermo-mechanical histories belongs to a part of the temperature-strain rate space, in which the model either was not trained or was trained on a small amount of homogeneously distributed data. Over 30% error in about 20% of points is likely related to this circumstance, however this requires more detailed analysis. The gaps in available data suggest what extra forging trials can be beneficial and how they should be designed. Fortunately, they are much cheaper and easier to conduct for the forging industry than lab tests.

The last thing that should be mentioned when talking about challenges relates to the fact that all the trajectories shown in Fig. 6 and used for training the model are obtained from FE simulations. Thus, the quality of this data and in turn the quality of the trained model is significantly dependent on the quality of the FE simulation.

Conclusion

This paper proposed a new approach to microstructure evolution modelling in hot forging processes using an AI-based model paired with a new methodology for data collection and model calibration using full thermo-mechanical histories acquired directly from industrial forgings with the use of FE simulation in QForm UK®.

An example of such a model has been made and calibrated using industrial hot forgings of two Double Truncated Cones made of Inconel 718. The model has been implemented into existing commercial metal forming simulation software as a user subroutine and blind tested on two complex disk forgings, showing the viability and high potential of the proposed approach.

Further development and implementation of AI-based models into industrial metal forming practice has the potential to increase the quality and reliability of microstructure evolution predictions compared to currently used models while making the process of calibrating such models drastically faster and cheaper.

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