COMPUTER METHODS IN MATERIALS SCIENCE

2021, vol. 21, no. 4, 209–218
https://doi.org/10.7494/cmms.2021.4.0769

A repeatability study of artificial neural network predictions in flow stress model development for a magnesium alloy

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Abstract

This work is devoted to an evaluation of the capabilities of artificial neural networks (ANN) in terms of developing a flow stress model for magnesium ZE20. The learning procedure is based on experimental flow-stress data following inverse analysis. Two types of artificial neural networks are investigated: a simple feedforward version and a recursive one. Issues related to the quality of input data and the size of the training dataset are presented and discussed. The work confirms the general ability of feedforward neural networks in flow stress data predictions. It also highlights that slightly better quality predictions are obtained using recursive neural networks.

Keywords: flow stress, artificial neural networks, feedforward, recursive

1. Introduction

Flow stress models (Pietrzyk et al., 2015) describe material behaviour during numerical simulations in terms of plastic deformation at different temperatures and strain rates. Flow stress data are most often determined by means of typical plastometric tests, e.g., uniaxial compression or tension. Standard flow stress models are based on closed-form mathematical equations where yield stress is described as a function of temperature, strain, and strain rate. The advantage of these approaches is the simple form of the mathematical function used to describe the flow stress evolution. However, conventional models do not take the influence of deformation history into account. Therefore, several more advanced flow stress models have been developed over the years, such as those based on internal variables (Roucoules et al., 2003). However, improving the predictive capabilities of models usually involves extending the computation time, especially when the finite element method is used for analysis. Therefore, there is a constant search for alternative approaches ensuring accuracy and acceptable computation time.

Data-driven flow stress models based on machine learning (ML) approaches have attracted increasing attention in recent years. ML is a group of approaches used in many different fields, e.g., to predict a protein's behaviour (Kozuch et al., 2018), design new materials (Curtarolo et al., 2013; Shi et al., 2019), or to predict the risk of delays in construction work (Gondia et al., 2020). An interesting application of ML is also presented in works by Pietrzyk et al. (2016), Mozaffar et al. (2019) and Stendal et al. (2018), which showed that it is possible to accurately predict materials' plasticity with deep learning approaches. ML approaches are primarily used as

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a substitute for time-consuming internal variable models or even complex multiscale approaches. However, ML can also be used to substitute the standard flow stress models when various deformation mechanisms (e.g. twinning, shear band development) control the deformation or when more complex deformation conditions (e.g. dynamic loading) are investigated. In such cases, the experimental data may not be sufficiently approximated by the mathematical formula (Deb et al., 2022).

Therefore, the current work aims to evaluate issues associated with the application of artificial neural networks (Baraniuk et al., 2020) to develop a flow stress model for magnesium ZE20 alloy. Computational models based on a deep learning algorithm recreate data at many abstraction levels (LeCun et al., 2015). The flow stress model in this research is being developed for a wide range of temperature and strain rate conditions.

2. Machine learning

Arthur Samuel is considered the founder of the term "machine learning" in 1959, defining it as computers' ability to learn without direct programming. ML is one of the essential sub-fields of artificial intelligence devoted to algorithms that learn from environmental data and stimuli, attempting in this respect to imitate human intelligence.

One of the basic machine learning solutions is artificial neural networks with an architecture inspired by the neuron structure of humans. As a result, the network consists of neurons aligned in layers that receive incoming stimuli, before selecting and developing an appropriate response. Neurons are connected, and there is a weight associated with each connection, as seen in Figure 1. The interpretation of these weights depends on the model of the neural network selected.

The crucial stage in neural network model development is the learning process. Learning is an algorithmic procedure that uses input data which the neural network uses to adapt its architecture to a given problem. The algorithm learns the patterns that occur, the relationships between the training set's values, and analyzes the obtained mathematical operations results. As an outcome, the model can find a solution to a given problem with a certain degree of probability. The algorithm processes the training data in the additional adaptation stage and learns from the mistakes (El Naqa et al., 2015). There are four main types of machine learning, including supervised learning – a learning process in which the training data results for a given data set are known. The algorithm learns by analyzing given results, detects dependencies in the input variables, and provides a probable response based on the analysis. The second type is semi-supervised learning – a learning process in which some of the training data results for a given data set is known. The third is unattended learning – the algorithm has no sample output for a given set of data. The neural network learns the patterns in the input data and predicts the output results. In this case, the accuracy of the obtained results increases with the training dataset size increase. Finally, the fourth variant is the reinforced type of learning. In this case, the neural network receives a set of permitted actions, statements, and rules as input information. Then it analyzes the results and effects of the performed actions.

A wide variety of different types of neural networks can be found in the scientific literature (Kiang et al., 2003; Lopez-Garcia et al., 2020). They can be divided according to learning method, the number of layers, type of the activation function, or signal distribution method. Two approaches were selected for the current investigation, the feedforward and recurrent ones.

3. Feedforward and recursive neural networks

The feedforward approach represents a basic type of neural network that is based only on a one-way direction signal processing (Fig. 2); therefore, they cannot include temporal dynamic effects.

The selected ANN was trained based on a set of experimental data obtained from a standard uniaxial compression plastometric test (Plumeri et al., 2019). The experimental data were obtained at a range of process conditions: T = 425°C, 400°C, 375°C, 350°C, 200°C and strain rates: 10 1/s, 5 1/s, 0.1 1/s, 0.01 1/s. Measured load-displacement data were then used to determine flow stress values based on the inverse analysis technique (Plumeri et al., 2019).

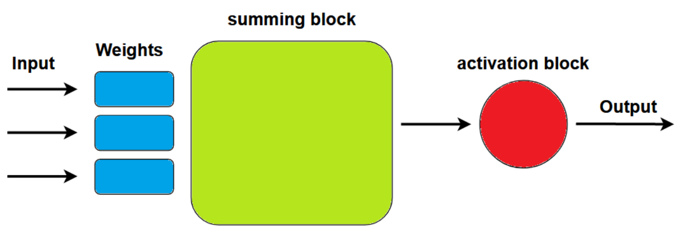

Fig. 1. Concept of an artificial neuron

In this manner, the quality of experimental input data is ensured as the inverse approach considers the influence of process heterogeneities, including friction or deformation heating, on flow stress data. However, to reduce the inverse analysis computing time, the number of input data is often reduced below 100 points for a particular flow stress curve. A set of flow stress curves used during the ANN development procedure is shown in Figure 3.

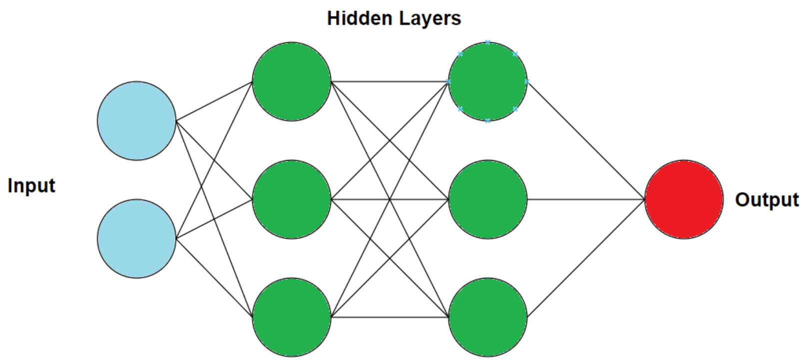

Fig. 2. Concept of the feedforward neural network

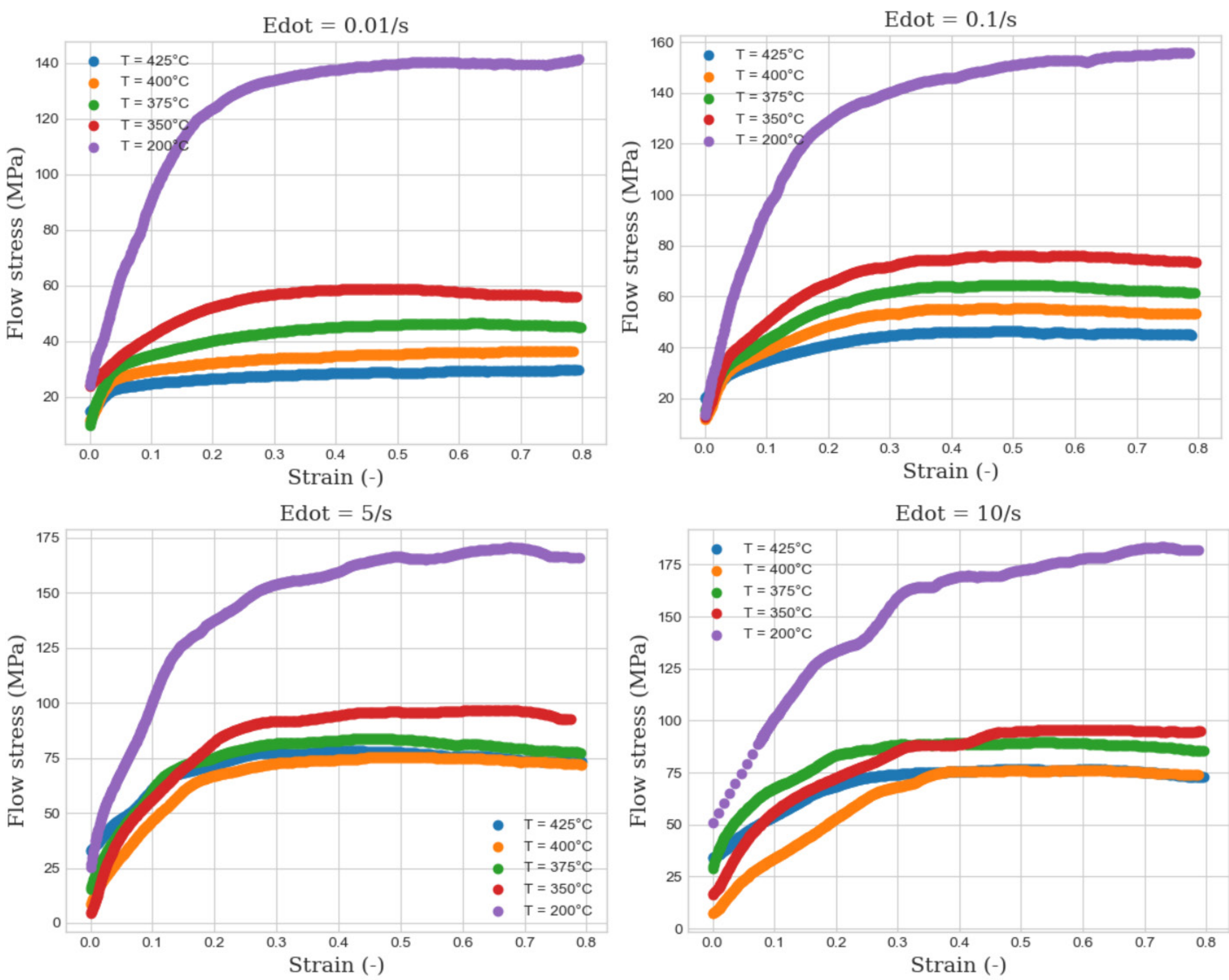

Fig. 3. Stress-strain curves determined based on experimental measurements and inverse analysis

An additional smoothing operation of the flow stress curves was performed with the data approximation technique to improve the training data set quality, as seen in Figure 4.

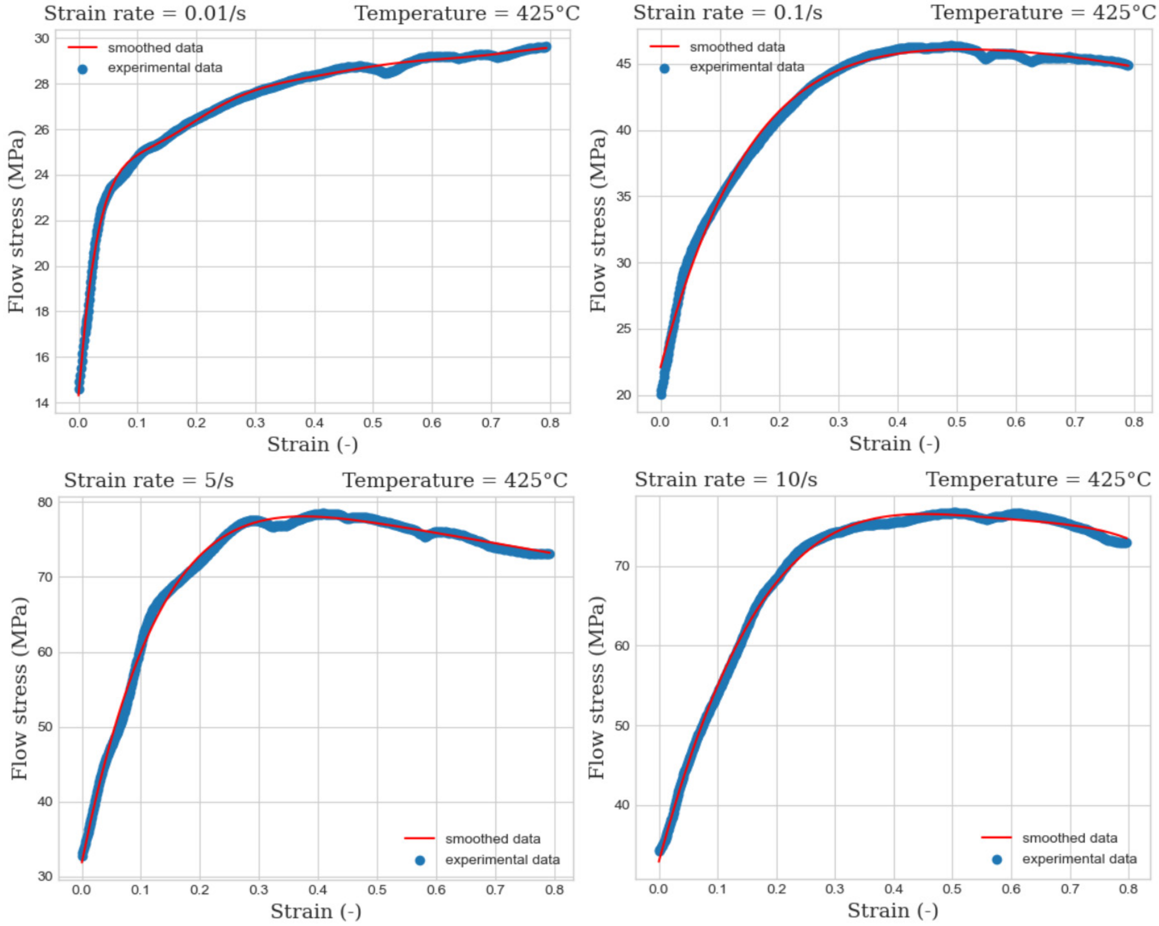

Fig. 4. Example of smoothed flow stress curves determined based on experimental measurements and inverse analysis for the T = 450°C

The 19 recorded stress-strain curves with approx. $L = 67$ points each were used to develop a first training dataset for the ANN. A separate set of stress-strain points with respect to the particular processing conditions $(T, \dot{\varepsilon})$ was used for the training. In that case, the training data set contains 1292 points $(\sigma_p, \varepsilon_i, T, \dot{\varepsilon})$. The selected stress-strain curve for $T = 375$°C and strain rate of 0.1 1/s was used to verify the results returned by the trained network. The ANN was initiated ten times to confirm the repetitive behaviour in the verification stage.

The sequential model, where each layer has exactly one input and output vector, with the rectified linear unit (ReLU) activation function (Xiang et al., 2021), was used for the investigations. The neural network structure was first developed on the basis of a trial and error procedure. A set of architectures was investigated based on shallow and deep neural networks (Stendal et al., 2019). It was found that in the investigated case, the best architecture consists of an input layer, an output layer, and two hidden layers with 32 and 16 neurons, respectively. The neural networks' training was based on the mean square error loss function (MSE) and RMSprop optimization algorithm (Lee et al., 2021).

At the same time, a more advanced ANN model based on a recursive algorithm (Khnissi et al., 2020) was also used for the investigation. Contrary to the feedforward artificial neural network, in which the flow of signals from the input to the output is unidirectional, the recursive neural networks introduce feedback loops, as illustrated in Figure 5. The same network setup parameters were used for feedforward and recursive ANNs.

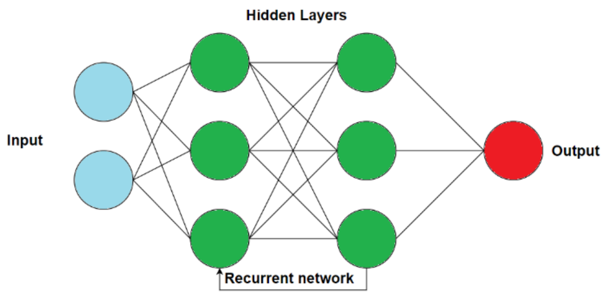

Fig. 5. Concept of the recursive neural network

4. Results and discussion

Both ANN types were used in the research under the concept of the supervised training approach. As already mentioned, the verification of the ANN behaviour also involved the repeatability of the predictions. For this, the ANN was initiated 10 times for each process condition. Obtained results for the feedforward and recursive neural networks training based on $L = 67$ are gathered in Figure 6. Based on these results, the best and the mean flow stress (average from all the cases) predictions were tested against the test data set as presented in Figure 7.

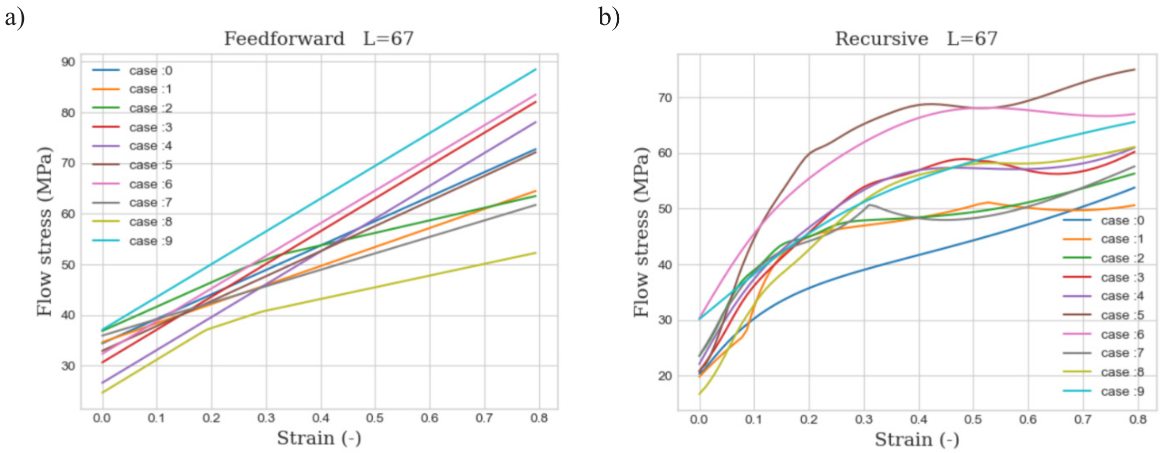

Fig. 6. Repeatability of the feedforward (a) and recursive neural networks predictions (b) for the training on the initial data set

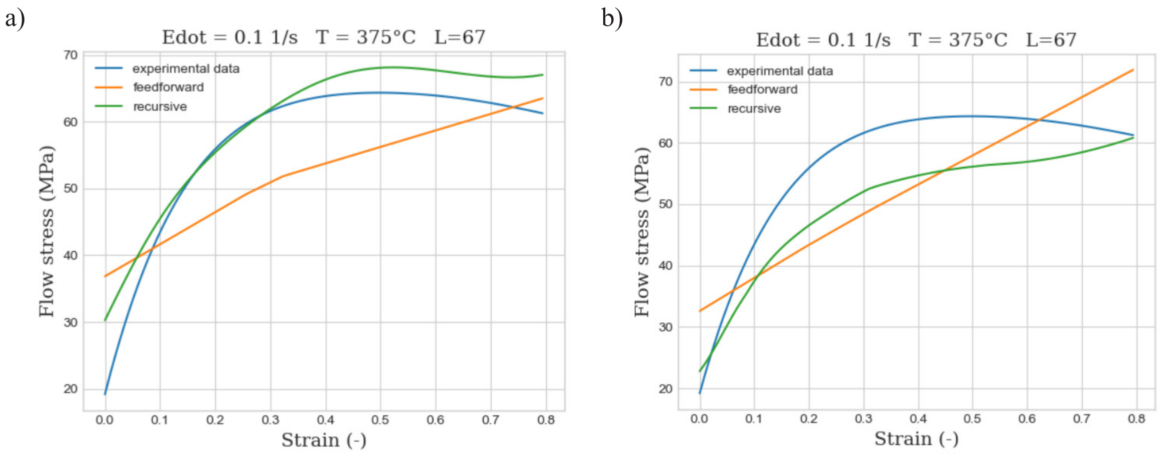

Fig. 7. Verification with the experimental data the best (a) and the mean (b) flow stress prediction

As presented, both the accuracy as well as the repeatability of flow stress curves for such a small training data set are unacceptable. Therefore, the number of training data was artificially augmented to improve the learning stage. In this case, an additional set of stress-strain points was generated as an average value of the two neighbouring original points. With that, the number of points in each stress-strain curve increased to L = 133, 265, 529 and 1057. That way, it is possible to evaluate how the ANN training process is affected by the number of training data points (Tab. 1). The training was done with the same ANN setup as previously. The repeatability results for subsequent case studies are collected in Figures 8 and 9.

Again for the testing purposes, the best and the mean predictions were compared against the test data set, as presented in Figures 10 and 11, respectively.

Table 1. Size of the training data sets

Number of points in a single flow stress curve L	133	256	529	1057
Number of points in the training data set T	2527	4864	10051	20083

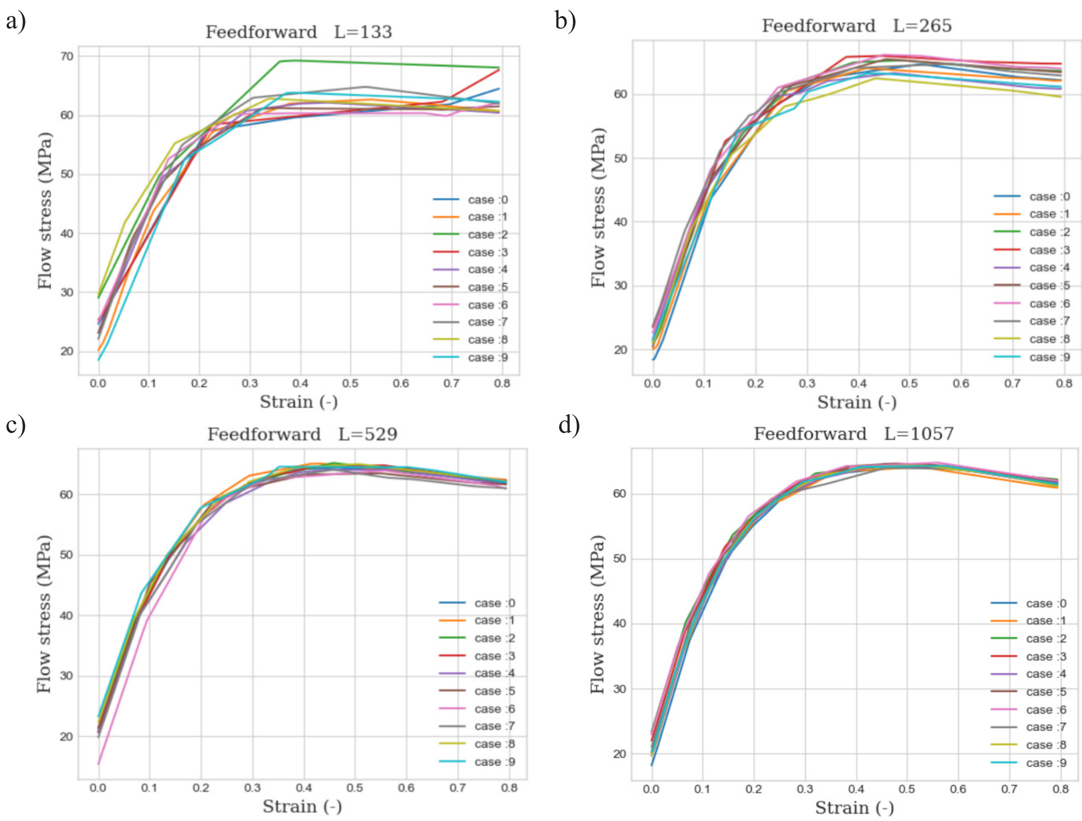

Fig. 8. Repeatability of the feedforward neural network predictions for the training on increasing data set size L: a) 133; b) 265; c) 529; d) 1057

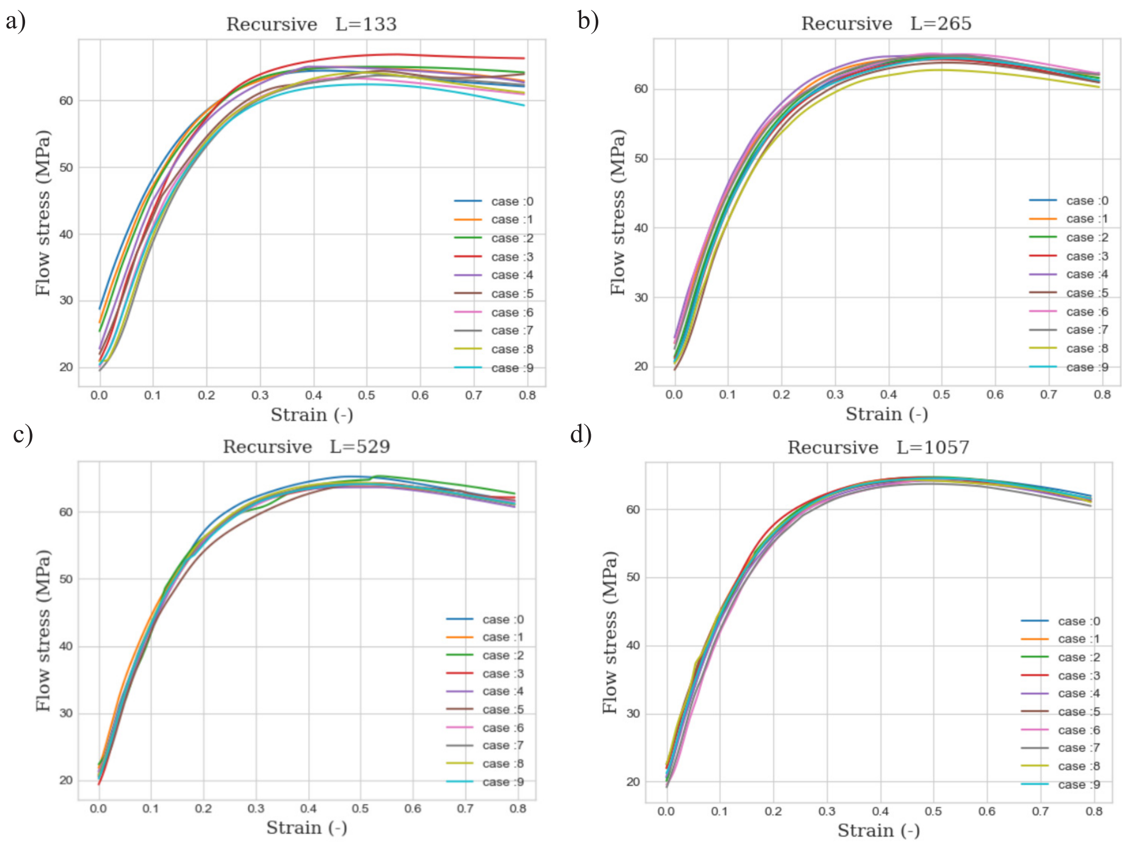

Fig. 9. Repeatability of the recursive neural network predictions for the training on increasing data set size L: a) 133; b) 265; c) 529; d) 1057

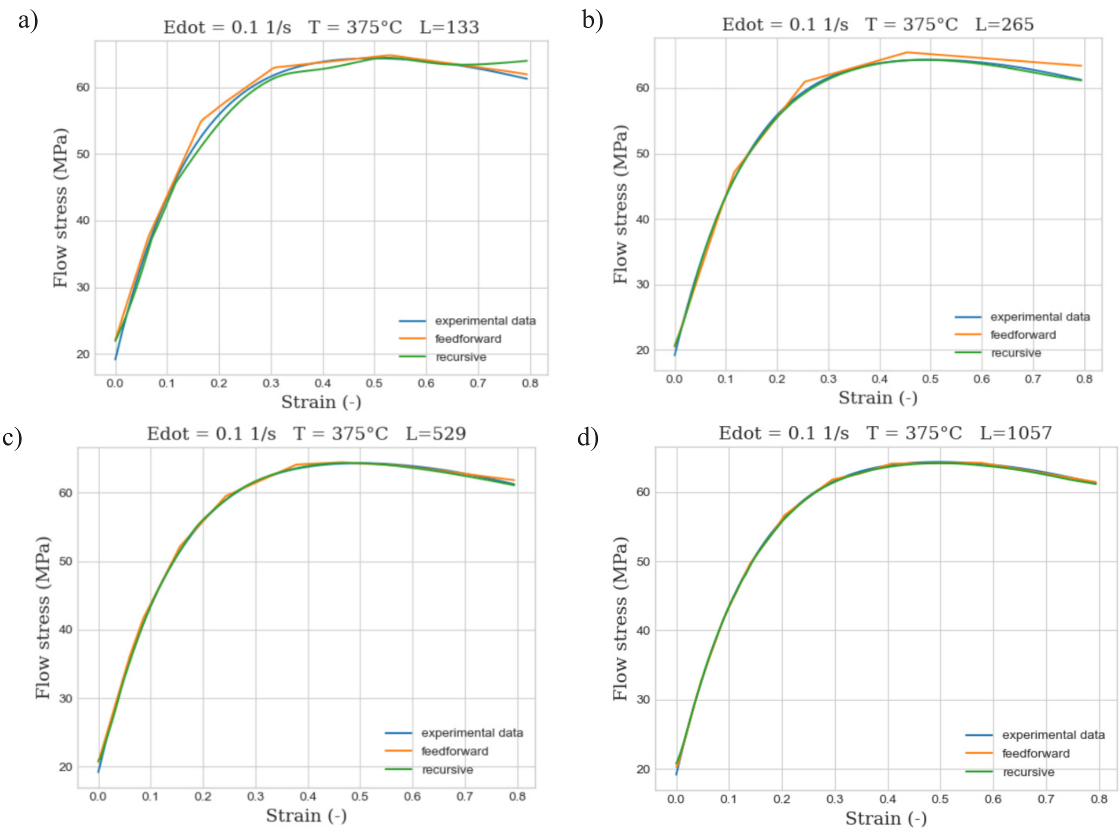

Fig. 10. Verification with the experimental data for the best predictions for the training on increasing data set size *L*: a) 133; b) 265; c) 529; d) 1057

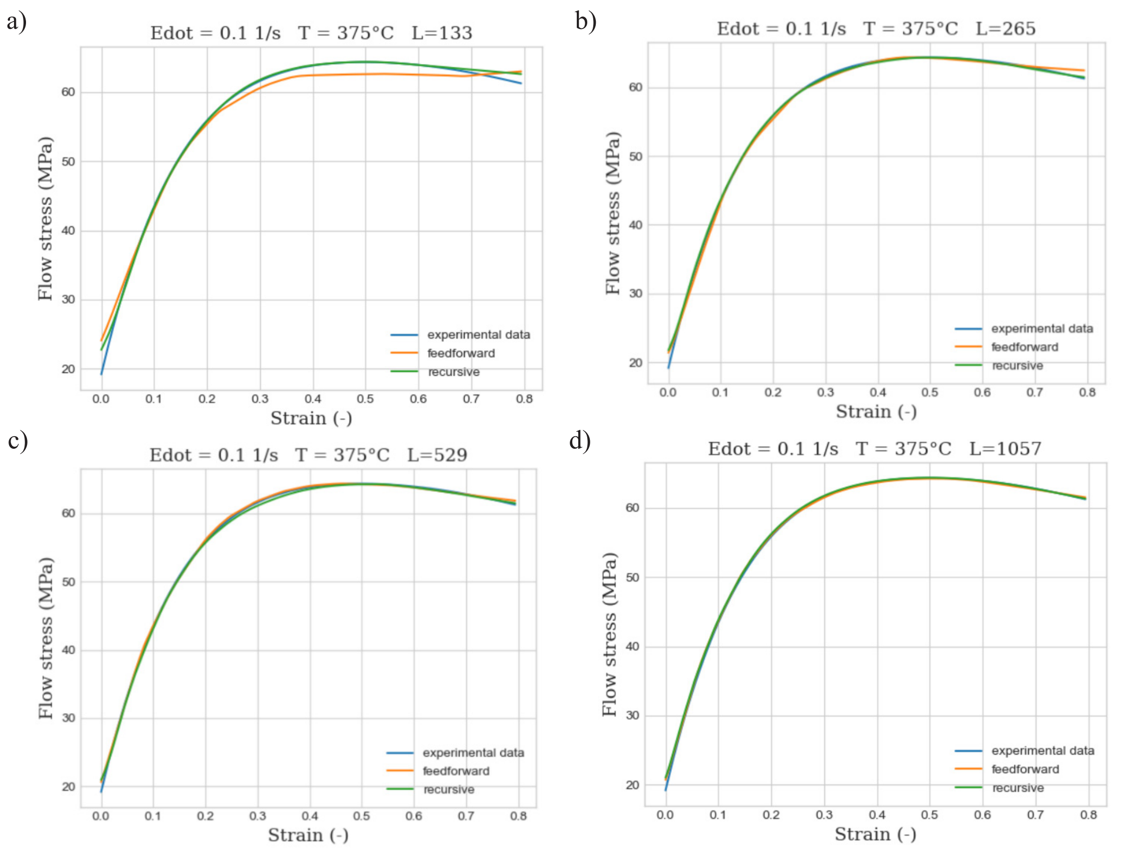

Fig. 11. Verification with the experimental data for the mean predictions for the training on increasing data set size *L*: a) 133; b) 265; c) 529; d) 1057

In the case of the best and mean flow stress curves, the recursive neural network already provides an acceptable solution for $L = 133$ training set, while the feedforward for $L = 265$. As seen, with an increasing number of points in the training data set, the repeatability of the predictions increases. However, the good repeatability of the predictions is obtained from the networks trained using the largest data set. In the case of the feedforward prediction, a typical step-shaped flow stress curve is predicted, which has to be treated as an artefact. When the mean value from several ANN runs is considered, this artefact is eliminated from the predictions, but it requires additional computational effort. Nevertheless, using mean values from several ANN predictions can increase the quality of the results in both feedforward and recursive neural networks. The results obtained also demonstrated that the training data set does not have to contain a huge number of training points. Therefore, if properly developed, both feedforward and recursive ANN can be used to generate flow stress data during, e.g., finite element simulations.

Conclusions

The obtained flow stress curves confirmed the effectiveness of the ANN algorithms in predicting the material behaviour under loading conditions in a wide range of processing conditions. In general, both feedforward and recursive ANN provide satisfactory results demonstrating a high level of repeatability. The repeatability of ANN predictions should be taken into account for practical use during finite element calculations, for example. An average value from several ANN runs should be used in this case. This is especially important for feedforward networks that have a tendency to predict stepped shaped flow curves. Therefore, the ANN can be used as a flow stress model of the ZE20 magnesium alloy for the finite element calculations, but the number of training data set has to be sufficiently large.

Future work will be focused on training the ANN, based on both stress-strain curves as well as the first derivative of the flow stress with respect to strain. Such an approach will then be used for the finite element simulation as a flow stress model.

Acknowledgement

The work was realized as a part of statutory research financed by the Ministry of Education and Science, grant no. 16.16.110.663.

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