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Neural network modelling of hot deformation of austenite

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Abstract: The hot deformation behaviour of austenite in steels is a complicated process which depends on chemical composition, microstructure, temperature and strain rate. While many models have been developed to represent the flow stress as a function of these variables, it is not yet possible to predict the behaviour for a new alloy. Linear regression techniques are not capable of representing the data, however, neural networks are capable of modelling highly non-linear data. A neural network model was developed in this work using a large database of various steels. The model allows the calculation of error bars that depend upon the position of a prediction in the input space and the level of perceived noise in the data. The validity of the model was evaluated by comparing its outputs against those of the six carbon-manganese steels with different compositions.

1. Hot deformation of metals

Hot-working often refers to deformation carried out under certain conditions of temperatures and strain rates so that the recovery and recrystallisation processes occur substantially in order to achieve large strains with essentially no strain hardening. Hot-working processes such as rolling are typically the first step in converting a cast ingot into a wrought product such as steel strips. Hot-working is usually carried out at a homologous temperature of 0.6 of the melting temperature and at strain rates between 0.5 and 500 s⁻¹ [1]. Laboratory tests for studying the metallurgical changes during hot-working are either hot-torsion or compression tests.

The general behaviour of a wide range of materials in response to increasing strain at high temperatures is rising the stress to a maximum value, followed by decrease to a steady-state flow stress, as shown in Figure 1.

There are two mechanisms responsible for softening in hot-working, depending on the metal [2]. In aluminium and alpha iron dynamic recovery is the softening mechanism. This occurs by the formation of a well-developed sub-grain structure by cross slip and climb, as occurs in creep deformation, and the activation energy for hot-working is that for creep and self-diffusion. In metals with a lower stacking fault-energy, the softening in hot-working is higher than for creep, and the softening occurs by the mechanism of dynamic recrystallisation. The difference in the stress/strain curves for the two types of materials are shown in Figure 1.

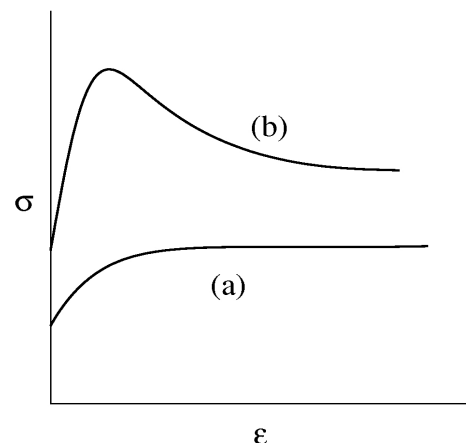


Fig. 1: Stress-strain curve for a metal exhibiting (a) dynamic recovery only; (b) dynamic recrystallisation after an initial period of dynamic recovery [1].

Dynamic recovery is the basic mechanism that leads to the annihilation of dislocations. This results

in a flow curve about one order of magnitude lower than in cold-working. The flow stress/plastic strain curve is essentially exponential, the stress rising to a steady state value when the work hardening and softening mechanisms are in equilibrium at higher strains. Low dislocation densities associated with the deformation are due to the ease of cross slip, climb, and dislocation unpinning. In metals that exhibit dynamic recrystallisation, dislocation annihilation only occurs when the dislocation density reaches high enough levels for recrystallisation to occur. As a result the flow stress rises to a peak value before dropping down to a steady state value where recovery and work hardening are in equilibrium.

2. Modelling of hot-working of steel

The vast majority of low alloy steels are shaped by hot-rolling and normally within the austenitic phase field where the upper limit of rolling temperature is governed by practical limitations associated with reheating and/or tooling. Common empirical models of hot-working of steel rely on mathematical representations of the flow stress versus the plastic strain behaviour of austenite, including the effect of strain rate and temperature, these are known as *constitutive equations*.

Whereas theoretical predictions can sometimes be made of simple properties such as the yield strength of a microstructure using dislocation theory and others, it is not yet possible to predict the strain-hardening coefficient [3]. The lack of progress in predicting the mechanical properties is because of their dependence on a large number of variables. Neural networks are extremely useful in these circumstances, allowing a quantitative expression of mechanical properties for complex problems where simplification leads to large errors.

There are many examples of neural networks applied to modelling the processes of hot-rolling, demonstrating the applicability of this approach. Singh *et al.* estimated the yield strength and tensile strength of steel as a function of 108 variables, including the chemical composition and an array of rolling parameters [4]. Korczak *et al.* used microstructural parameters as inputs to calculate ferrite grain size and property distributions [5]. There are also many examples of modelling the mechanical properties of steels. Dumortier *et al.* have modelled the properties of micro-alloyed steels [6], Millytoski has published many papers about modelling various properties of steels including the hot torsion of austenite and a comparison of the models with physical models [7, 8].

The work presented here uses a neural network with a Bayesian framework. This approach was used to predict flow stress from the inputs of composition, temperature, strain rate and strain. The Bayesian approach to neural networks makes predictions with error bars, with the magnitude depending upon the position in the input space and perceived level of noise in the model. This should be extremely useful from an industrial point of view. Often, when data are needed to optimise processing schedules of a new steel, the processing conditions are not readily available, and it is unclear to what extent the conditions used for other steels can be exploited. As a result constitutive data often need to be generated by a large number of tests for each steel with a new composition.

3. Basis of neural network modeling

Neural networks are statistical models of real world systems, built by tuning a set of parameters known as *weights*. The weights make up a model, which represents a mapping from the input values to the output values. The weights are calculated by passing examples of input-output pairs through the model, and adjusting the weights to minimise the error or prediction, with appropriate measures to avoid overfitting.

There are two major tasks that neural networks can be applied to: classification and continuous

numeric functions. Classification refers to variables which take in only 0 or 1 values. It is the continuous numeric functions that are of the most relevance to modelling of constitutive behaviour. Neural networks represent a general method of regression that can overcome some of the difficulties associated with ordinary linear regression, such as the need to choose the form of any relationship between the parameters before analysis. The artificial neural network arrives at a mathematical model without prior assumptions about the form of the relationships. Relationships in the neural network are not limited to the sum of linear or pseudo-linear terms.

Bayesian probability theory provides a unifying framework for data modelling which offers several benefits. Overfitting can be avoided by using methods to control model complexity, while probabilistic modelling handles uncertainty in a natural manner [9].

Using neural networks within a Bayesian framework allows uncertainties of fitting to be estimated in a manner which depends upon the region of the input space where the prediction is calculated. Instead of calculating a unique set of weights, a probability distribution of sets of weights is used to define the fitting uncertainty. This methodology is extremely useful when applied to problems in materials science where properties need to be estimated as a function of a large number of inputs, which are not uniformly distributed in the input space [3].

Neural networks can create functions with much more flexibility than ordinary linear regression. Figure 2 shows a typical function produced using a neural network with two inputs and one output; in contrast the function produced by a linear regression would be a flat plane [9].

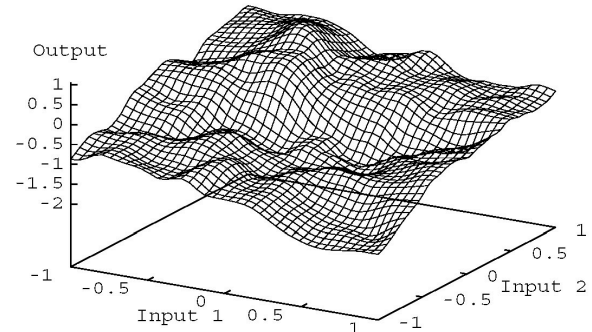


Fig. 2: Typical function produced by neural network. [9]

The final output, y , is defined as:

$$y = \sum w_i^{(2)} h_i + \theta^{(2)} \quad \text{Eq. 1}$$

where

$$h_i = \tanh \{ \sum w_{ij}^{(2)} x_j + \theta_i^{(1)} \} \quad \text{Eq. 1b}$$

and x_j are the j variables on which the output y depends, w_i are the weights, θ and θ_i are the biases.

The form of the relationship described by equation 1 is interesting. A hyperbolic tangent function (Eq. 1b) is used to operate the weights inputs because such a function is non-linear and flexible in the sense that its shape is dependent on the weights. Combining several hyperbolic tangents together gives even greater flexibility so that the complexity of the model is also related to the number of hyperbolic tangent operators used. It is important that complexity be penalized, so that the appropriate trends can be automatically extracted from the training data. More details on the mathematical aspects of neural networks modeling are given elsewhere [10,11,12].

Review of previous neural network models used to predict constitutive behaviour: Previous work has demonstrated the ability of neural networks in modelling constitutive behaviour. Narayan *et al.* [13] has demonstrated that hot-torsion stress/strain curves can be represented using a neural network technique, even taking into account the deformation history of the material. Hwu, *et al.* [14] developed a neural network for prediction of flow stress using data from six steels, they reported that their neural network model could interpolate flow stresses very well but the capability for extrapolation was not impressive. An attempt was made to build results from linear regression

for carbon equivalence into the model and they found that this lowered the quality of the training. Kong and Hodgson and co-workers have integrated constitutive and neural network models reporting significantly improved accuracy of predictions with changes in chemical composition [15]. The integrated model they developed predicted the parameters of the Estrin–Mecking model from the input parameters of carbon content, temperature, strain rate, Zener–Hollomon parameter and activation energy. Liu *et al.* [16] compared using neural networks with the use of the Zener–Hollomon parameter and hyperbolic sine stress function to model the behaviour of high-speed steel. Dimitriu and Bhadeshia have modelled the hot strength of creep-resistant ferritic steels [17]. The applicability of neural networks to materials science problems in general has been made clear in reviews by Bhadeshia and Bhadeshia *et al.* [18,19].

4. Data acquisition and results of modelling

The experimental data were provided by Corus (Swindon Technical Centre-UK) including constitutive data describing the behaviours of low, medium, and high carbon steels, carbon-manganese steels, high strength low alloy steels, and austenitic steels.

The data were in the form of stress/strain data. Typically the tests had a maximum strain of 0.7, the hot-working temperatures of 700-1200°C, and with the strain rates varying from 0.01 to 100 s⁻¹.

The compositions of the 24 steels used in training the neural network model are listed in Table 1. The amount of information about the compositions of each alloy varied, since the data were collected from various sources, rather than being generated by a systematic test program designed specifically for the purposes of neural network analysis. The data are from

commercial grades of steel, rather than alloys designed to extract information about the physical behaviour of steels, with some variation in composition. Data for a further 6 steels were collected from published work and compositions of these steels are shown in Table 2 [20]. These results were used to demonstrate the predictive abilities of the model.

The first model produced used the data without trying to give the model any physical basis. One aim of this model is to look for trends in the data, another was to decide which data points should be included in later models. The phosphorus and sulphur data were left out to simplify the model since they are “tramp” elements usually present at similar levels.

Table 1: Chemical compositions of the alloys used to train the network.

Alloy	Composition (wt%) balance Fe							
	C	Si	Mn	Cr	Ni	Mo	Cu	V
78C_railsteel	0.780	0.230	0.850	0.013	0.011	0.010	0.023	–
50Concast	0.180	0.300	1.320	0.015	0.019	0.001	0.011	0.080
55Concast	0.150	0.200	1.300	0.019	0.020	0.001	0.018	0.150
43Concast	0.200	0.240	1.210	0.022	0.023	0.004	0.023	0.001
100C	1.000	0.190	0.170	0.100	0.090	–	–	–
55C	0.560	0.360	0.280	0.120	0.090	–	–	–
15C_A	0.147	0.270	0.480	0.070	0.099	–	0.275	–
En16	0.350	0.270	1.490	0.030	0.110	0.280	–	–
En31	1.060	0.220	0.460	1.410	0.170	–	–	–
En52	0.470	3.740	0.580	8.200	0.200	–	–	–
VniCu	0.090	0.307	1.430	0.020	0.223	0.003	0.324	0.132
En45	0.610	0.940	1.580	0.120	0.270	0.060	–	–
En40	0.260	0.570	0.350	3.030	0.290	0.490	–	–
En25	0.350	0.270	0.660	0.590	2.540	0.590	–	–
304	0.070	0.430	0.480	18.600	7.700	–	–	–
316	0.070	0.670	1.340	17.290	12.040	2.260	–	–
20C	0.190	0.040	0.860	–	–	–	–	–
16C_V	0.160	0.260	1.220	–	–	–	–	0.064
95C	0.960	0.087	0.910	–	–	–	–	–
25C	0.250	0.080	0.450	–	–	–	–	–
12C	0.120	0.200	0.050	0.080	–	–	0.100	–
Leaded steel	0.078	0.003	1.220	–	–	–	–	–
08C	0.087	0.003	0.340	–	–	–	–	–
45C	0.430	0.260	0.740	–	–	–	–	–

Table 2: Chemical compositions of the alloys used to show the predictive power of the model.

Alloy	Composition (wt%) balance Fe		
	C	Si	Mn
Steel1	0.010	0.150	0.190
Steel2	0.030	0.320	0.620
Steel3	0.190	0.310	0.640
Steel4	0.380	0.340	0.640
Steel5	0.590	0.640	0.350
Steel6	0.900	0.730	0.460

Once the data were collected and stored they were then normalized. A number of sub-models were selected and trained; these differ in the initial number of hidden units and starting weight values. The data was randomised and split into a training set and a testing set. Figure 3 compares one predicted stress-strain curve against the experimental values.

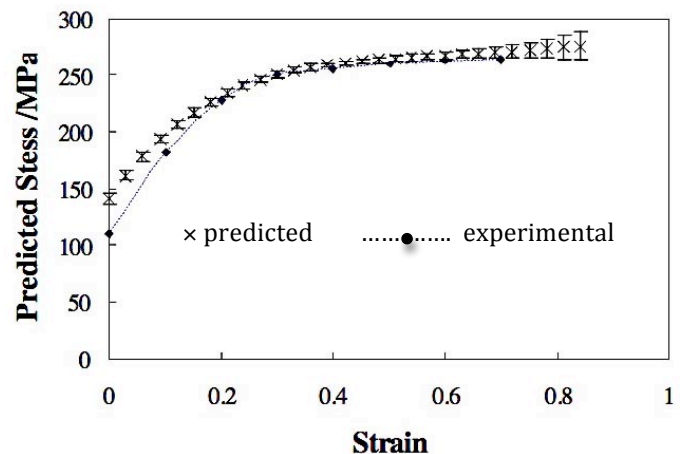


Fig. 3: Stress vs. strain in Grade 25C steel at temperature 800°C, and strain rate of 30 s⁻¹.

Figure 4 shows the performance of one of the models developed in this work in predicting the stress vs. strain in the six steels listed in Table 2. Steels 1-4 data are from compression tests at temperatures from 700 to 1200°C and strain rates from 0.5 to 140 s⁻¹. Steels 5 & 6 data are from the same temperature range but at strain rates of 2 s⁻¹ and 20 s⁻¹ only. The results are encouraging since some stresses are correctly predicted, especially those with the temperature and strain rate within the range of the training data. The predictions that differ widely from the experimental values are usually accompanied by large error bars. However some of the predictions have negative values of stress, and this has to be recognised as a “nonsense” prediction. These large variations from the experimental values were expected for steels 1 & 2 at low temperatures. This can be explained by the possibility of ferrite formation in steels 1 & 2, and hence represents predictions away from the experience of the model, which only contains data for the austenitic region.

A more physically based neural network was developed by presenting the database with more meaningful inputs, simplifying the task of finding the appropriate trends in the data. Each element was incorporated as the (natural) logarithm of the corresponding at.%. The other inputs were the logarithm of the strain and strain rate and the output was the logarithm of the stress. This resulted in improved performance over the first model.

5. Conclusion

- A neural network model has been produced capable of reproducing and predicting the flow stress during hot deformation of austenite, and is available for download [21].
- Neural networks are a general form of regression, and the results demonstrate how they are more appropriate than traditional linear regression techniques, because in physical systems the effect of changing one variable depends also on the values of the other variables. For example in hot working the effect of changing carbon content depends upon the temperature and strain rate.
- The quality of the neural network is highly dependent on the quality of the dataset.
- The compositions available for training meant the neural network was limited in its applicability to the 8 elements of carbon, manganese, silicon, chromium, nickel, vanadium, copper, and molybdenum. It has been proved that the applicability of this kind of model to a larger database would further improve the results and extend the range of validity, especially since micro-alloying elements such as niobium have an effect on flow stress response during hot working.
- Predictions can interpolate and extrapolate the stress-strain behaviour of austenite in hot rolling, the confidence in the prediction is indicated by the magnitude of the error bars.

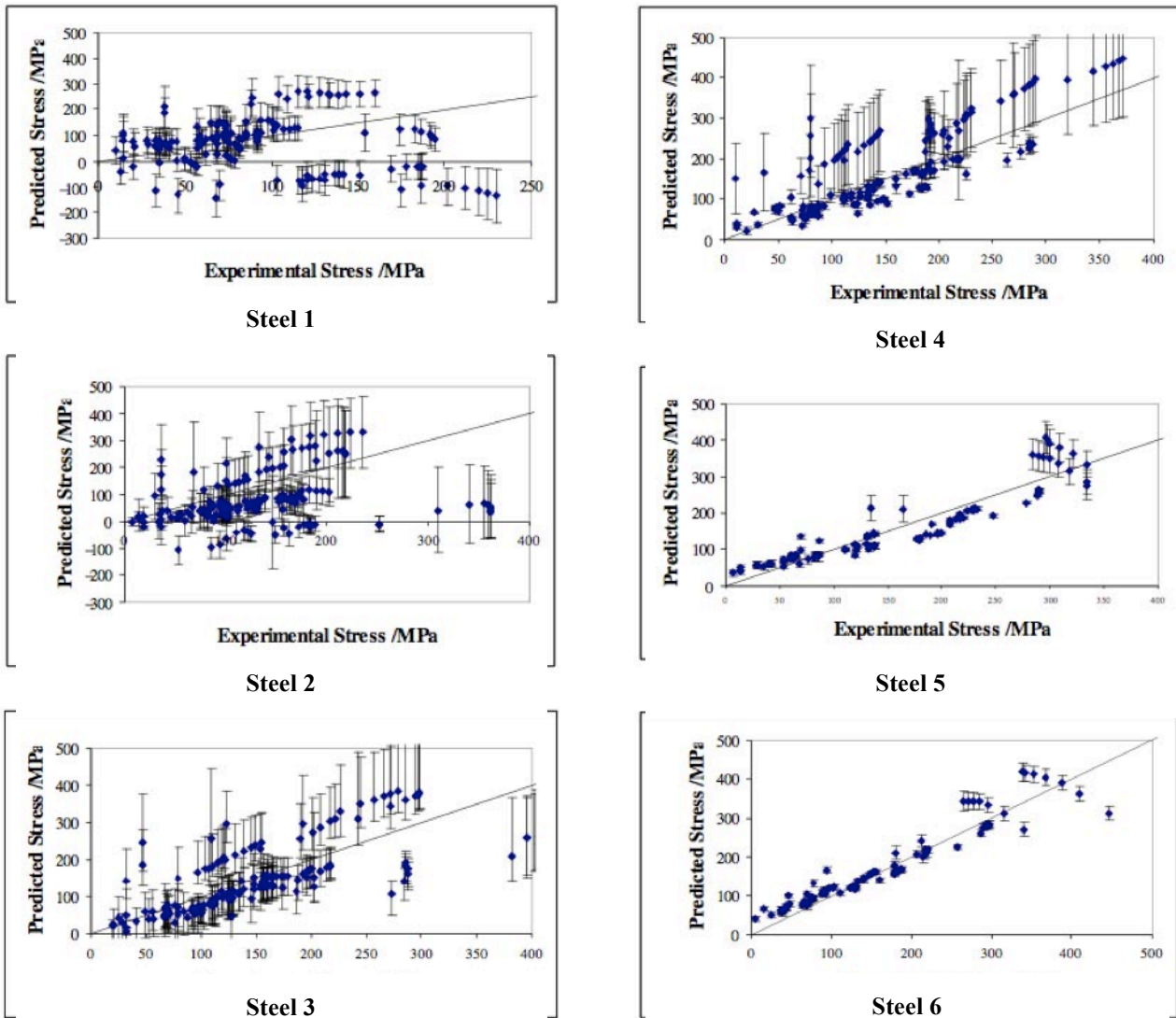


Fig. 4: Flow stresses predicted by the neural network model for six steels listed in Table 2 are compared with corresponding experimental data (see the text for test conditions).

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