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Estimation of deformation induced martensite in austenitic stainless steels

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ABSTRACT

The extent of deformation induced martensite (DIM) is controlled by steel chemistry, strain rate, stress, strain, grain size, stress state, initial texture and temperature of deformation. In this research, a neural network model within a Bayesian framework has been created using extensive published data correlating the extent of DIM with its influencing parameters in a variety of austenitic grade stainless steels. The Bayesian method puts error bars on the predicted value of the rate and allows the significance of each individual parameter to be estimated. In addition, it is possible to estimate the isolated influence of particular variable such as grain size, which cannot in practice be varied independently. This demonstrates the ability of the method to investigate the new phenomena in cases where the information cannot be accessed experimentally. The model has been applied to confirm that the predictions are reasonable in the context of metallurgical principles, present experimental data and other recent data published in the literatures.

1. Introduction

Austenitic stainless steels are extensively used in engineering applications, nuclear power plant components, automobile and pharmaceutical industries due to their excellent corrosion resistance, weldability and mechanical properties. Metastable austenitic stainless steels undergo DIM transformation, where the γ (fcc) austenite is transformed to thermodynamically more stable α' (bcc) martensite due to plastic deformation. This phase transformation enhances the work hardening of these steels, and affects their ductility [1].

Furthermore, the microstructural evolution and the mechanical behaviour are sensitive to chemical composition, temperature, stress, strain, strain path, strain rate, stress state, grain size, and initial crystallographic microtexture. Understanding the influence of these factors, resulting microstructures and the corresponding mechanical behaviour are the most important part not only in terms of the selection of the best material, but also in the optimal development of material models, which are nowadays extensively applied in the automobile and nuclear power plant industries to understand their forming and crash related performances. Considerable attention was given in the past to the microstructure of austenitic stainless steels, the stability of the phases present in these steels and the effects of amount and distribution of the phases present on the mechanical behaviour of the material under service. The mechanical properties of metastable austenitic stainless steels are strongly influenced by the morphologies and the extent of deformation induced phase transformation.

In the past, there has been a constantly increasing interest for neural network modelling in different fields of materials science [2]. Several models have been developed for prediction of mechanical properties, phase transformations, optimizing alloy composition, processing parameters, heat treatment conditions, on line corrosion monitoring, improving weldability, etc. [2]. This empirical approach becomes more attractive as it is fairly the robust technique and in most cases, it rapidly converges to a target solution. This provides a range of powerful new techniques for solving problems in pattern recognition, data analysis and control.

The purpose of the work presented here is to develop a model, which makes possible the estimation of DIM content as function of its influencing variables using neural network technique within a Bayesian framework [3]. This model would tremendously help to the nuclear power plant, automobiles and pharmaceutical industries to design their components under service. In the present context, the optimization process needs access to a quantitative relationship between the chemical composition of austenitic stainless steels, grain size, stress, strain, temperature, strain rate and the ultimate the extent of DIM. A neural network method has been developed to correlate those and applied extensively for applications.

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Table 1
Statistics of database used for neural network analysis. SR: strain rate, T: temperature, GS: grain size, TSS: true stress, TSN: true strain, DIM: deformation induced martensite and SD: standard deviation. The column marked 'Example' is a specific case used to generate Fig. 14.

Inputs	Units	Maximum	Minimum	Mean	SD	Example
C	wt%	0.10	0.007	0.05	0.03	0.028
Mn	wt%	8.92	0.42	1.761	1.61	1.32
Cr	wt%	18.58	15.40	17.78	0.68	18.13
Ni	wt%	13.53	2.75	8.03	1.59	8.32
Mo	wt%	2.53	0	0.31	0.53	0.15
N	wt%	0.24	0	0.05	0.05	0.044
Cu	wt%	0.70	0	0.16	0.15	0.26
Nb	wt%	0.11	0	0.006	0.016	0.015
Co	wt%	0.20	0	0.042	0.07	0.10
Ti	wt%	0.67	0	0.01	0.08	0.01
SR	s^{-1}	200	0.0001	6.44	34.74	0.000125
T	°C	200	−196	−1.49	66.79	24
GS	μm	200	5.90	29.19	28.16	23.8
TSS	MPa	1951.17	14.22	848.33	282.78	1078.33
TSN	–	0.65	0	0.25	0.14	0.37

Output	Units	Maximum	Minimum	Mean	SD
DIM	–	1	0	0.22	0.24

2. Results and Discussion

2.1. Analytical procedure

We have extensively carried out literature study to understand the martensitic transformation micro-mechanisms and their interpretation while explaining the mechanical behaviour of austenitic stainless steels under various operating conditions. For the present model, inputs are chosen according to the knowledge gained from the published literatures and from the industrial experiences. The inputs of the model are chosen to be: chemistry of austenitic stainless steels, strain rate, initial austenite grain size, temperature of testing, true stress and true strain. The target (i.e. output) is the extent of DIM. The other influencing parameters for martensitic transformations are stress state, initial microtexture of austenite and strain path, which were not, included as input parameters because there is lack of published data available. In most of those literatures, we considered those studies, which deal with different grades of austenitic stainless steels with different grain sizes under uniaxial loading at various testing conditions. In most of those literatures, DIM is generally represented as strain induced martensite. Various techniques have been used for quantifying the DIM formation in those literatures, such as: XRD, magnetic methods etc. The most common and available graphs are found to be: (a) stress–strain and (b) DIM as a function of strain. We have extensively extracted data (i.e. strain, DIM fraction and corresponding stress value) from those two graphs with their corresponding testing conditions and material history reported in corresponding literatures. We have tabulated all the data in a single spreadsheet and the size of the database, which are used for neural network analysis to be 1600 rows. The literatures (1954–2010), from where those data digitized are mentioned to be [1,4–27]. The statistics of the whole database are given in Table 1. It is emphasised that unlike linear regression analysis, the ranges stated in Table 1 cannot be used to define the range of applicability of the neural network analysis. This is because the inputs are in general expected to interact each other. We shall see later that it is the Bayesian framework of our neural network analysis, which makes possible the calculation of error bars whose magnitude varies with the position in the input space, which define the range of useful applicability of the trained network. A visual impression of the spread of the data is shown in Fig. 1(a–o).

2.2. Empirical modelling

A neural network is a general method of regression analysis in which a very flexible non-linear function is fitted to the experimental data. It can capture the enormous complexity in the database, which avoid over fitting [28]. It is nevertheless useful to discuss some salient features, to place the technique in the context. The Bayesian framework of neural network has been used in this present study. A neural network is generally trained on a set of examples of input and output data with repetitive representations. The outcome of training is a set of co-efficient (i.e. weights) and a specification of the functions, which in combination with the weights correlating the inputs to the output. The training process itself involves a search for the optimum non-linear correlation between the inputs to the output and is computer intensive. Once the neural network is trained, the estimation of the output for any given inputs is very easy. The details of this method used here have recently been comprehensively reviewed by MacKay [29] and the original method is described thoroughly elsewhere [29–34]. One of the difficulties with the blind data modelling is that of over fitting, in which spurious details and the noise in the training data are over fitted by the model. This gives rise to solutions that generalise poorly. MacKay [29–34] and Neal [35] have developed a Bayesian framework for neural networks in which the appropriate model complexity is inferred from the database. This Bayesian neural network modelling has two important advantages. Firstly, the significance of all the input variables is quantified automatically, which is extremely important to understand the response of each variable. Consequently, the model perceived significance of each input variable can be compared against the existing metallurgical theory. Secondly, the neural network's predictions are accompanied by error bars, which depend on the specific position in input space. This quantifies the model's certainty about its predictions. In this present study, both the inputs and output variables were first normalised within the range ±0.5 as follows:

$$x_N = \frac{x - x_{min}}{x_{max} - x_{min}} - 0.5 \quad (1)$$

where x_N is the normalised value of x; x_{min} and x_{max} are respectively the minimum and maximum values of x in the entire dataset (Table 1). The normalisation is straightforward for all the quantitative variables. The normalisation is not necessary for this analysis but facilitates the subsequent comparison of the significance of