Review

Neural networks in materials science
H.K.D.H.Bhadeshia

There are difficult problems in materials science where the general concepts might be understood but which are not as yet amenable to scientific treatment. We are at the same time told that good engineering has the responsibility to reach objectives in a cost and time-effective way. Any model which deals with only a small part of the required technology is therefore unlikely to be treated with respect. Neural network analysis is a form of regression or classification modelling which can help resolve these difficulties whilst striving for longer term solutions. This paper begins with an introduction to neural networks and contains a review of some applications of the technique in the context of materials science.

Mechanical Properties

Statistical modelling of mechanical tensile properties of steels by using neural networks and multivariate data analysis
C.Dumortier et al.

Both Neural networks NN and Multivariate Data Analysis MDA techniques were used to determine mechanical tensile properties of steels. NN apparently proved better in dealing with non-linearity effects and complex interactions between the predictors. However, MDA was found essential in improving the quality of the prediction and providing interpretation to the results from NN modelling.

Petri neural network model for the effect of controlled thermomechanical process parameters on the mechanical properties of HSLA steels
S.DATTA et al.

The effect of composition and controlled thermomechanical process parameters on the mechanical properties of HSLA steels is modelled using the Widrow–Hoff's concept of training a neural net with feed-forward topology by applying Rumelhart's back propagation type algorithm for supervised learning, using a Petri like net structure. The data used are from laboratory experiments as well as from the published literature. The results from the neural network are found to be consistent and in good agreement with the experimented results.

The application of constitutive and artificial neural network models to predict the hot strength of steels
L.X.Kong et al.

Many constitutive models have been successfully used to interpolatively and extrapolatively predict the hot strength of metal materials and artificial neural network (ANN) models have recently appeared to be an alternative for constitutive modelling due to the strong capability of the ANN in predicting and correlating nonlinear relationship between inputs and outputs. In this work, the constitutive and ANN models will initially be used to predict the complex stress strain behaviours of an austenitic steel with carbon content ranging from 0.0037 to 0.79 wt%. Due to the limitations of the models and the complexity of the material properties, both the constitutive and ANN models cannot accurately predict the effect of chemical composition. As both models have their advantages, the integration of constitutive and ANN models significantly improves the prediction accuracy and the complex influence of the chemical composition is more accurately predicted.

Estimation of hot torsion stress strain curves in iron alloys using a neural network analysis
V.Narayan et al.

The hot torsion stress-strain curves of steels have been modelled using a neural network, within a Bayesian framework. The analysis is based on an extensive database consisting of detailed chemical composition, temperature and strain rate from new hot torsion experiments. Non-linear functions are obtained, describing the variation of stress–strain curves with temperature and chemical composition. Predictions are associated with error bars, whose magnitude depends on their position in the input space. From the population of possible models, a "committee of models" is found to give the most reliable estimate. The results from the neural network model where found to be consistent with known models, and reasonable estimates are obtained beyond the scope of the experimental data.

Application of neural networks to mechanical property determination of Ni-base superalloys
J.Warde et al.

In this work the application of a neural network, within a Bayesian framework, to the prediction of tensile properties has been critically assessed. Following optimisation of input parameters a series of neural networks were trained to predict tensile properties of a range of polycrystalline superalloys as a function of temperature.

Once trained the models have been subjected to several metallurgical tests in order to demonstrate that they predict the trends expected from experimental observations. Generally it is found that the models are in agreement with expected trends. In addition areas of uncertainty are highlighted through the production of large error bars, which act as warning signals.

Use of neural networks for alloy design
J.Warde et al.

This paper demonstrates the application of a neural network model to an alloy design process for a Ni-base polycrystalline superalloy. The network model used had the ability to predict tensile properties for polycrystalline superalloys as a function of temperature and chemical composition.

Given set mechanical property targets and compositional limits it is possible to use the model to narrow down the choice of potential composition to those combinations which achieve or exceed the set levels. This process can dramatically reduce the number of melts that would need to be produced in an experimental process. Further considerations such as TCP formation or cost can be combined with this method, to further contract the number of alloy compositions requiring production for evaluation purposes.

Through such an approach a more cost-effective and rapid alloy development route has been demonstrated.

Comparison of artificial neural networks with Gaussian processes to model the yield strength of nickel-base superalloys
F.Tanklet et al.

The abilities of artificial neural networks and Gaussian processes to model the yield strength of nickel-base superalloys as a function of composition and temperature have been compared on the basis of simple well-known metallurgical trends (influence of Ti, Al, Co, Mo, W, Ta, of the Ti/Al ratio, γ' volume fraction and the testing temperature). The methodologies are found to give similar results, and are able to predict the behaviour of materials that were not shown to the models during their creation. The Gaussian process modelling method is the simpler method to use, but its computational cost becomes larger than that of neural networks for large data sets.

Data pre-processing/model initialisation in neurofuzzy modelling of structure–property relationships in Al–Zn–Mg–Cu alloys
O.P.Feminnella et al.

The paper deals with the application of multiple linear regression and neurofuzzy modelling approaches to 7xxx series based aluminium alloys. 36 compositional and ageing time variants and subsequent proof strength and electrical conductivity measurements have been studied. The input datasets have been transformed in two ways: to reveal more explicit microstructural information and to reflect some empirical findings in the literature. Neurofuzzy modelling exhibited improved performance in modelling proof strength and electrical conductivity cf. the multiple linear regression approach. Electrical conductivity is best modelled using the explicit microstructural input dataset, whilst proof strength is best modelled by a further modification of this dataset, decided upon after inspection of the subnetwork structures produced by neurofuzzy modelling. Neurofuzzy modelling offers a transparent empirically based data-driven approach that can be combined with pre-processing of the data and initialising of the model structure based upon physical understanding. An iterative modelling approach is defined whereby data-driven empirical modelling approaches are first used to assess underlying data structures and are validated against physically based understanding, these then inform subsequent initialised neurofuzzy models and input data transformations to provide both optimal subset and feature representation.

Phase Transformations

Effects of carbon concentration and cooling rate on continuous cooling transformations predicted by artificial neural network

J. WANG et al.

Employing 151 continuous cooling transformation (CCT) diagrams, an artificial neural network (ANN) has been modeled and trained. The CCT diagrams of a class of Fe–xC–0.4Si–0.8Mn–1.0Cr–0.003P–0.002S (x within 0.1 through 0.6) steels are predicted by the model developed. It indicates that an increase in carbon concentration (C%) gives rise to a decrease in ferrite start (Fs), bainite start (BS), and martensite start (MS) temperatures, but the carbon concentration has weak effect on the pearlite end (Pe) temperature. The rate of decrease, $\partial Fs/\partial C$, further depends on the carbon concentration. The carbon dependence predicted by ANN is consistent with what is predicted by thermodynamic models. The Fs temperature is also affected by the cooling rate (v), especially for high carbon steels and v>0.1°C/s. C prolongs the incubation period of ferrite formation, but accelerate the overall growth kinetics of the pearlite reaction. The Fs and Pe temperatures at low cooling rates predicted by the ANN model are in agreement with those predicted by thermodynamic models. The deviations of Pe and Fs from their thermodynamic equilibrium counterparts are nearly independent of the carbon concentration. The minimum undercooling for both ferrite and pearlite reactions is around 50°C. It increases up to 100°C at higher cooling rates. Pre-bainite decomposition of austenite retards bainite formation. Employing the Ms temperature, the critical driving force for heterogeneous athermal nucleation are also estimated and related to the Ms temperature. Ms temperatures predicted by this model prove to be consistent with those predicted by several empirical linear models. It can be concluded that the current ANN model is reliable and effective.

System Control

Forecasting heat levels in blast furnaces using a neural network model

Y. OTSUKA et al.

Heat level is one of the important factors influencing the stable operation of blast furnaces, and it is especially important to accurately forecast decreasing heat levels in order to stabilize the heat level.

A forecasting model for decreasing heat levels which occur accompanied with a sudden rising of wall temperatures has been developed using neural network technology. Wall temperatures are measured at various points in the vertical and circular directions. Temperature rising points are measured as a distributed pattern, and neural network technology is used in order to recognize this distributed pattern.

Neural network models are classified into two groups according to their learning style, one is called the supervised learning model and the other, the unsupervised learning model. The operators notice that a decrease in heat level sometimes occurs after a rise in wall temperature, but there is no knowledge of what patterns cause the heat level decrease, which means there is no teaching data for the supervised model. The forecasting model is built using one of the unsupervised neural network models, the self organization feature maps model, which recognizes and classifies the wall temperature rising patterns. A new method of shift invariant recognition has been developed in order to put circularly shifted wall temperature rising patterns together in a class.

It has been established that the heat level forecasting model using the classified wall temperature pattern gives better forecasting accuracy for heat level decrease than a forecasting model using the total amount of wall temperature rising points. Furthermore, this heat level forecasting model, which uses a classified wall temperature pattern and solution loss C, has sufficient accuracy for heat level operation guidance.

Mold level control in continuous caster by neural network model

T. WATANABE et al.

In continuous billet casting, keeping the mold level steady is one of the most important technologies for maintaining steel quality. Using conventional methods, it is difficult to attain precise control of the mold level because of the nonlinear characteristics of the process. We have developed a control system using a neural network model to overcome this problem. In this paper, control problems of a continuous caster are introduced first. Next, the structure of the control system is proposed. In our proposed system, the neural network model recognizes the temporal patterns of inlet flow and controls the stopper stroke for a main control loop with a PI controller. The problems involved in construction of a valid neural network model that has good generalization and robust properties, are discussed from the viewpoint of optimizing the number of hidden layer units by the information criterion. Finally some results of its application are described.

Welding

Application of neural networks for quality evaluation of resistance spot welds

U. DILTHEY et al.

A neural network based system was developed to perform non-destructive quality evaluation of spot welds. The spot welds are classified with a high reliability of 100 %, taking variations of the welding parameters and electrode wear into account. The classification was carried out by the means of preprocessed data from the course of welding current and voltage.

Using AI-methods for parameter scheduling, quality control and weld geometry determination in GMA-welding

U. DILTHEY et al.

At the ISF-Welding Institute at Aachen University neural networks have been used for some years, for developing effective quality control systems of GMA welding. Also artificial intelligence methods are applied to recognise the quality and to calculate the seam geometry (seam height and thickness). In addition the neural networks are used as target functions for genetic programming in order to find out an optimised welding parameter set.

Primary welding parameters and statistically evaluated transient signals of the welding process are taken as an input data record for a neural network.

Since it is very time consuming to obtain a comprehensive information about the quality of the whole weld beat by evaluating numerous metallographic images, a software tool which calculates the beat geometry from the data supplied by a laser scanner, has been developed.

Recognition rates of neural networks between 90 and 100% have been achieved for short and pulsed arc processes in online quality control and in offline parameter optimisation. The error in the geometry prediction by the neural network was found to be within the range of 2–12%.

Measurement of molten pool shape and penetration control applying neural network in TIG welding of thin steel plates

Y. SUGA et al.

An intelligent welding robot system with visual sensors is developed in order to realize full automatic welding of thin mild steel plates including automatic seam tracking and automatic control of welding conditions. A system to detect the shape and dimension of molten pool using CCD camera and a penetration control system using Neural Network in TIG arc welding are investigated. In order to characterize the shape of molten pool, width, length and area of the molten pool were measured, and are used to form the contour of the molten pool as shape parameters. These parameters are input to the neural network, which outputs optimum welding conditions to control the penetration of the molten pool. Consequently, if unexpected changes occur in welding conditions, such as root gap, welding speed and so on, the welding system can optimumly control the welding conditions. The constructed system is tested and found to be effective for penetration control in automatic butt welding of thin mild steel plates.

Application of artificial neural network to discrimination of defect type in automatic radiographic testing of welds

K. AOKI et al.

The X-ray radiographic testing method is often used for detecting weld defects as a non-destructive testing method (NDT). Due to the difficulties in identifying small defects from the X-ray film, skilled laborers should be trained. However, recently it has been difficult to employ skilled laborers. Moreover, for the identification process, not only the laborers skill influence the testing result, but also it is difficult for skilled laborers to assess small flaws within a short time. In comparison, computer visual image processing system have some good characteristics, allowing objective assessment, high speed judgment, non-human's error etc. Therefore, an image processing system allows weld defects to detect using X-ray radiography in the presence of background noise. This paper deals with an image processing method for displaying defects by computer graphics. Furthermore an application of neural network to discriminate the type of defect was tried. As the result of the investigation, it was seen that the system constructed is effective to the detection and discrimination of small weld defects clearly.

Neural networks applied to welding: Two examples

J.M. Vitek

Neural network analysis provides for a powerful means for non-linear regression analysis that can be applied to a wide variety of problems. This paper describes the application of neural networks to two welding areas. The general approach for the development of the back propagation neural networks is described, including the method that was used to identify the optimum neural network architecture and the best neural network. The first application considers the weld profile shape in pulsed laser aluminum welds and the prediction of the profiles as a function of weld process conditions. It is shown that the neural network predictions are reasonably accurate in most cases, in spite of the fact that the training data set was quite small. The second application considers the prediction of Ferrite Number in stainless steel welds as a function of weld composition. For this application an extensive training data set was available. The neural network that was developed was compared to conventional means for predicting Ferrite Number and it was shown that the neural network was considerably more accurate than other currently available methods.

A neural network approach to the prediction of submerged arc weld metal chemistry

R.C. Thomson et al.

A neural network technique has been employed to predict submerged arc weld metal chemistry, using a database for which a previous linear regression model had been developed. Thus, a comparison may be made of neural network and regression approaches. Weld metal chemistry is a complex function of interactions between the welding electrode, baseplate and shielding medium. It is demonstrated that simplifying assumptions made in the regression analysis, *i.e.* that the final weld metal composition is largely dependent on the plate and wire chemistries, are justified when the dataset is restricted to similar weld process variables. However, for a wider range of flux chemistries, for example, the neural network recognises the more complex interrelationships within the data. Similarly, complex models are generated by a neural network to predict properties such as weld metal toughness for which a simple relationship between input variables can not be derived.