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Modelling correlation between alloy composition and ferrite number in duplex stainless steel welds using artificial neural networks

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Weld metal composition is thought to be an important factor in influencing the austenite/ferrite ratio of duplex stainless steel microstructures. To produce the required balance in the austenite/ferrite ratio in the weld microstructure, the chemical composition of the welding consumables should be adjusted. In the present work, Bayesian neural network analysis has been employed to predict the ferrite number in duplex stainless steel welds as a function of composition. The technique accounts for modelling uncertainty, and automatically quantifies the significance of each input variable. In this paper, the influence of variations in the weld composition on the ferrite number have been quantified for two duplex stainless steels. Predictions are accurate compared to published methods. The role of Si and Ti in influencing the ferrite number in these alloys has been brought out clearly in this study while these elements are not given due considerations in the WRC–1992 diagram.

Keywords: Artificial neural networks, Duplex stainless steel welds, Ferrite number

Introduction

Duplex stainless steels, in comparison with conventional austenitic and ferritic stainless steels, have a two phase microstructure containing approximately equal amounts of austenite and δ ferrite. They possess an excellent combination of properties, some of which are superior to austenitic stainless steels. They are therefore being considered for applications in the temperature range 253–573 K, such as in chemical process equipment, pollution control devices, marine applications, and particularly for tubing in oil and gas wells.[1,2]

The ferrite:austenite (F:A) ratio influences the mechanical, chemical, and electrochemical properties of duplex stainless steel weldments. The yield and ultimate tensile strengths of the welds are not greatly affected by the extended ferrite number (EFN) over the very wide range 32–117 EFN,[3] and as long as the ferrite content exceeds 30 EFN the strength properties of the weld are similar to that of the base metal. However, the ductility and notch toughness are markedly affected by the ferrite content, and ferrite content less than 60 EFN is necessary to ensure integrity. While ferrite content less than 35% results in a deterioration of stress corrosion resistance, ferrite content exceeding 60% is detrimental to cracking resistance due to reduced toughness and increased susceptibility to hydrogen assisted cracking and pitting.

Obtaining similar corrosion and mechanical properties across a duplex stainless steel weldment is not possible by the common practice of using matching composition filler and base metals, because appreciably higher ferrite content is obtained in the weld than in the base metal as both chemical composition and thermal history affect the F:A balance. As it is difficult to control the thermal characteristics during welding, the required F:A balance in duplex stainless steel welds can be achieved by adjusting the chemical composition of the welding consumable.[4–6]

FN is generally assessed using the WRC-1992 diagram,[7,8] which does not include[9] Si, W, and Ti. It also does not adequately address the effects of cooling rate. The method relies on linear relations, which may not be justified.[10] Neural network analysis involves non-linear regression analysis[11,12] and hence is better suited to complex cases involving many possibly interacting variables.[13]

In neural network analysis, the data are presented to the network in the form of input and output parameters, and the non-linear relationships are found by minimising the difference between measured and predicted values. The results consist of a series of coefficients and a specification of the type of function that, in combination with weights, relates the inputs to the

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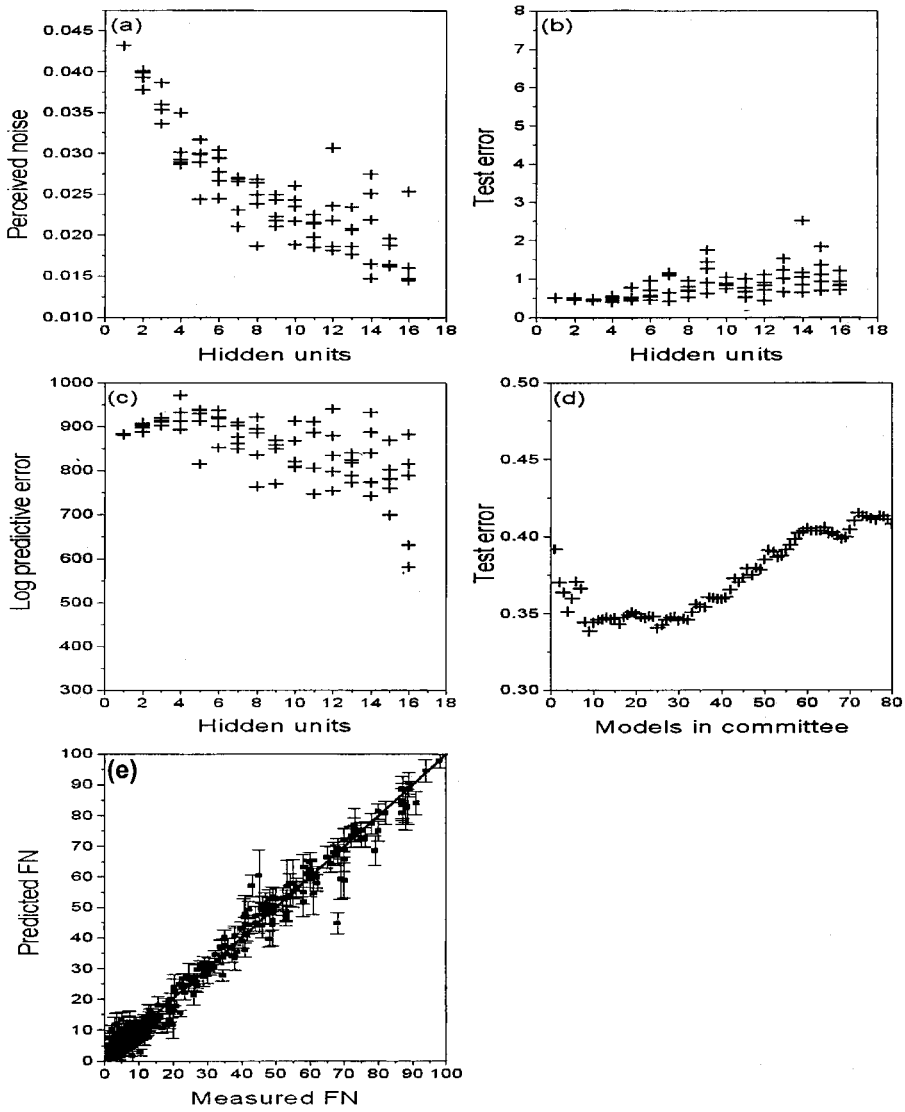


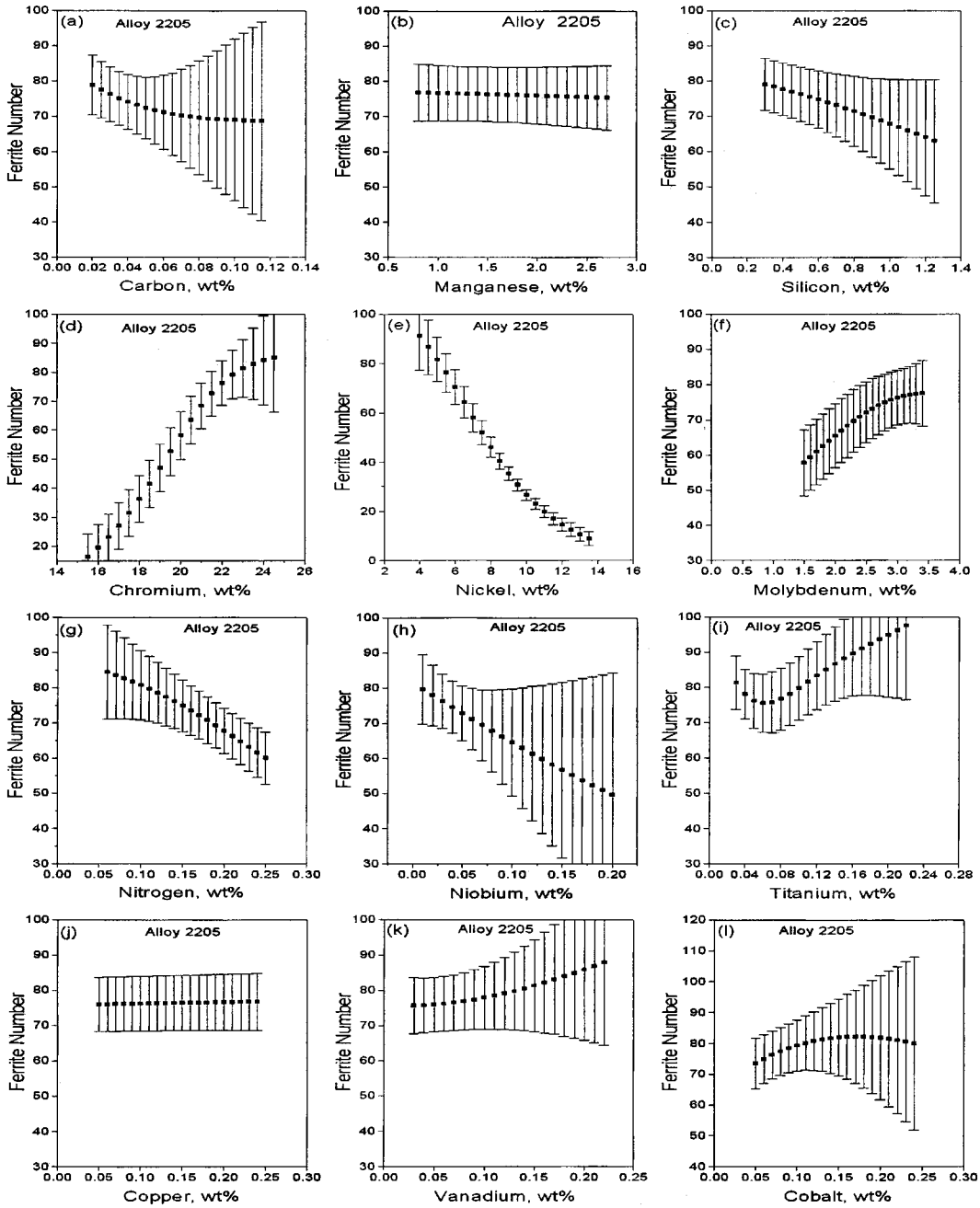
a noise versus hidden units; *b* test error versus hidden units; *c* predictive error versus hidden units; *d* test error versus models in committee; *e* predicted FN versus measured FN predicted using optimum committee of models for the entire 1020 datasets

1 Characteristics of BNN model for FN prediction

output. To prevent overfitting, a Bayesian framework has been developed by controlling the complexity of the neural network.[14] This framework, which has been extensively used to model the mechanical properties of welds and FN in stainless steel welds,[15–19] has been used for predicting FN to a higher accuracy than other available FN prediction methods.[20] In this paper, the characteristics of this model are briefly described and used to study the influence of weld chemistry on the FN in two widely used duplex stainless steel welds.

Table 1 Range, mean, and standard deviation of composition variables (input) and ferrite number, FN (output)

Elements	Minimum value	Maximum value	Mean	Std. deviation
C	0·0000	0·2000	0·0401	0·0218
Mn	0·3500	12·6700	1·8506	1·7334
Si	0·0300	6·4600	0·5295	0·3383
Cr	1·0500	32·0000	20·4822	2·7230
Ni	4·6100	33·5000	11·2636	2·5964
Mo	0·0100	10·7000	1·4770	1·5520
N	0·0100	2·1300	0·0857	0·1006
Nb	0·0100	0·8800	0·0435	0·0905
Ti	0·0100	0·3300	0·0348	0·0285
Cu	0·0200	6·1800	0·1470	0·4139
V	0·0300	0·2300	0·0588	0·0228
Co	0·0100	0·6900	0·0519	0·0410
Fe	45·5990	72·5150	63·9784	4·2206
FN	0·0000	98·0000	12·5140	18·0225



a C; *b* Mn; *c* Si; *d* Cr; *e* Ni; *f* Mo; *g* N; *h* Nb; *i* Ti; *j* Cu; *k* V; *l* Co

2 Predicted FN for alloy 2205 duplex stainless steel weld with different concentrations of elements (concentration of other elements held constant except for Fe, which is adjusted to compensate for the concentration varying element)

Database

The Bayesian neural network model has been developed using 1020 datasets of shielded metal arc (SMA) weld compositions and ferrite contents for 300 series austenitic stainless steel and duplex stainless steel welds. Of the 1020 datasets, 948 data are those used to generate the WRC–1992 diagram,[21] and the remaining datasets are from in house laboratory experiments. When variables such as Nb, Ti, V, Cu, and Co, were not available, they were set to the average over the entire dataset. The assumed values of these elements were (in wt-%) Nb=0·03; Ti=0·022; Cu=0·02; V=0·04; Co=0·035. These values represent only the residual concentration levels of these elements. This was found to be better than the assumption of a value of zero for these elements as was used in an earlier model.[18,19] The range, mean, and standard deviation of each composition variable (input) and the FN value (output) are given in Table 1. Although Table 1 shows the range of compositions covered, they cannot be used to define the range of applicability of this BNN model as the input variables are expected to interact in this neural network analysis. Instead, error bars were used to define the range of useful applicability of this BNN model.

Bayesian neural network (BNN) analysis

The BNN analysis has been extensively used for modelling and predicting the mechanical properties of welds and for alloy design; a complete description of which is available elsewhere.[14] The aim here is to model

for the FN in stainless steel welds as a function of composition, with the networks employed consisting of 13 input nodes x_i representing the 13 composition variables, a number of hidden nodes h_i, and one output node y representing the FN value. Both the input and output variables were normalised within the range $\pm 0{\cdot}5$. Eighty different models were created with the number of hidden units varying from 1 to 16, in which five different sets of random seeds were used to initiate each network for a given number of hidden units. These were trained using a training dataset comprising a random selection of one-half (i.e. 510) of the total 1020 datasets, while the remainder were used as the test dataset to examine how the model generalises with unseen data. The details of the Bayesian neural network analysis, such as activation function and uncertainties, are described elsewhere.[18,20]

Results and discussion

Characteristics of the Bayesian neural network (BNN) model for FN prediction

The characteristics of the model are detailed in Fig. 1, which shows that the perceived noise σ_v decreases with increasing number of hidden units (Fig. 1*a*). The test error has a minimum at four hidden units (Fig. 2*b*), and the log predictive error (*LPE*) attains a maximum at four hidden units (Fig. 2*c*). The error bars throughout this work represent a combination of σ_v in the output and the uncertainty in fitting estimated from the Bayesian framework.

A committee of models can make more reliable predictions than an individual model, with the best models being ranked based on their *LPE* values. A committee of models is formed by combining the predictions of the best L models, with the size of the committee given by the value of L, and a plot of the test error of the committee versus its size (Fig. 1*d*) shows a minimum that defines the optimum size of the committee. Figure 1*d* also shows that the test error associated with the best single model is clearly greater than that of any of the committees. In this work, a committee with nine models was found to have the optimum membership with the least error and, therefore, this committee was retrained on the entire dataset and used for subsequent predictions. The comparison between the predicted FN and measured FN values for this optimum committee is shown in Fig. 1*e*. Good correlation was observed between the predicted and measured FN values. The correlation coefficient obtained was 0·98, which is better than for any of the currently available FN prediction methods.[12]

The generalised BNN model for FN prediction[20] also revealed the significance of individual elements on the FN value. It was found that the FN value was influenced insignificantly by Mn and Nb, most significantly by Cr, Ni, Mo, and N, and less significantly by C than by N. More importantly, it was found that the elements Si, Ti, V and Co also significantly influence the FN value, elements which are not included in the WRC–1992 diagram.

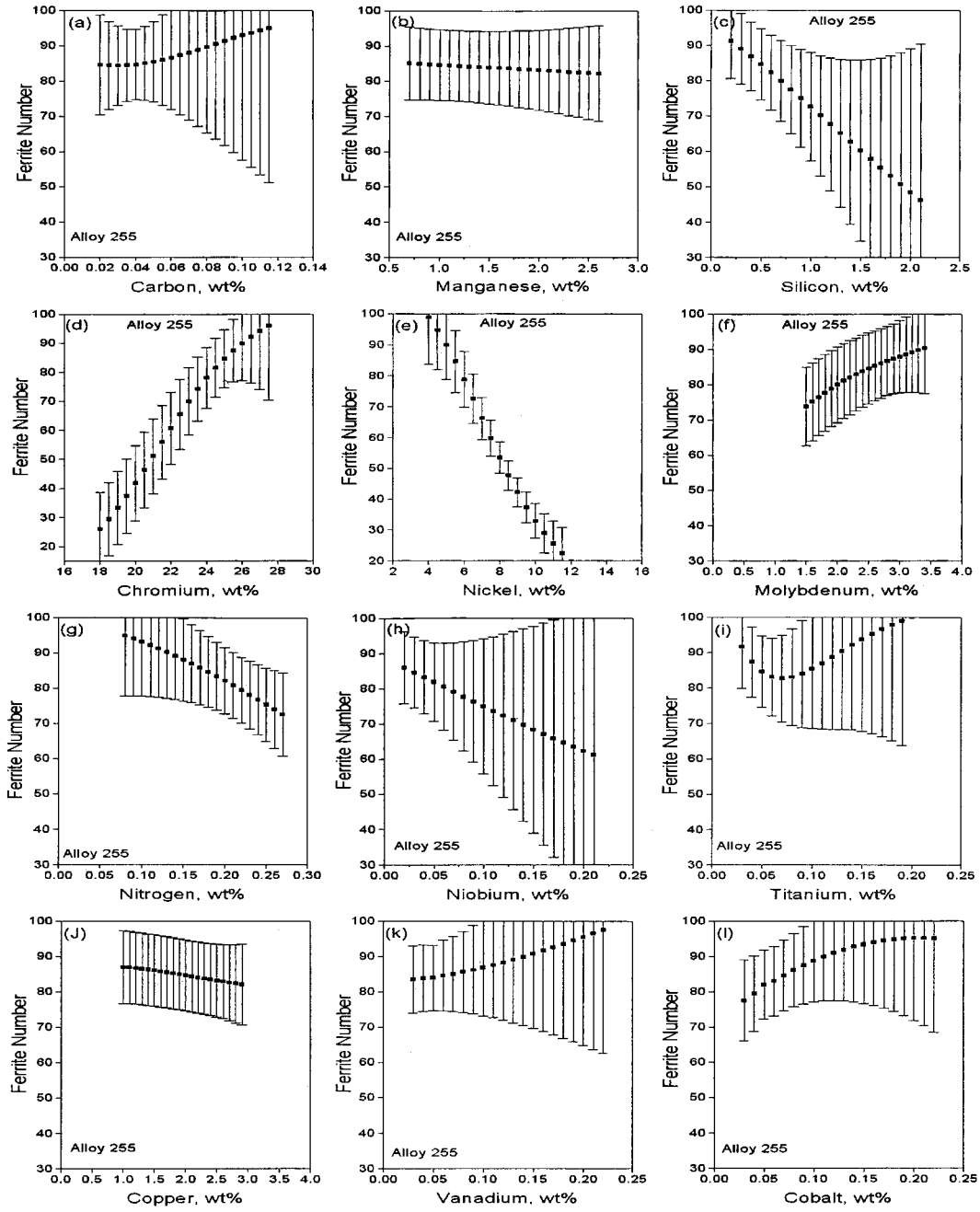
Composition dependence of FN value in duplex stainless steel

A major limitation of the WRC-1992 diagram is its linearity, so that the influence of individual elements on the FN value remains constant irrespective of any change in base alloy composition. As neural networks can incorporate interactions between the input variables, it is possible to model. The trained network was used to study two different duplex stainless steels (Table 2).

Figure 2 shows the influence of concentration on the FN value for 12 elements in alloy 2205. Error bars representing the uncertainty in prediction are included. The size and shape of the error bar in each figure depends on the distribution and noise of the training dataset used. It was found that C, Ni, and N act as austenite stabilisers, with N having a stronger effect than C. This is in agreement with the results reported by Vitek *et al.*[12] Although the Mn content in the training dataset varied from 0·5 to 1·98 wt-% for duplex stainless steel welds, the variation in Mn content was found not to influence the FN. The observation that variation in Mn does not influence the FN is in agreement with that reported by Szumachowski and Kotecki[22] for austenitic stainless steel welds. Also Mn was removed from the Ni_{eq} calculation when the WRC-92 diagram was proposed.[21] In alloy 2205, Si and Nb were also found to stabilise austenite. The observation that Si is an austenite stabiliser is in agreement with that reported by Suresh Babu *et al.*[23] In the present BNN model, in which average Nb concentration of 0·03% over the entire dataset is assumed, shows that Nb acts as an austenite stabiliser. However, one would expect Nb to tie up with C and N and by reducing their content in austenite it should be a ferrite stabiliser. But that is not observed here possibly because Nb is not effective in forming carbides and nitrides at this low concentration and in the presence of V and Ti, which are also strong carbide and nitride formers. Large error bars observed for Nb concentrations greater than 0·05% imply that prediction is uncertain and more experiments are necessary. However, the trend predicted by the model is valid. The FNN-1999 model, in which Nb content was assumed to be zero (as it was not available), reports that variation in Nb concentration does not influence the FN value.[12] Figure 2 also shows that Cr, Mo, and V act as ferrite stabilisers, while Ti and Co have varying effects. Titanium acts as an austenite stabiliser at low Ti contents $<0{\cdot}05\%$, but acts as a strong ferrite stabiliser at Ti contents $>0{\cdot}05\%$ due to the formation of nitrides that remove the potential austenitising effect of N. At low concentration levels Ti is not effective in forming carbides and nitrides and so C and N remain in austenite and that in turn stabilises the austenite. Ti

Table 2 Chemical composition of two sample duplex stainless steel base compositions, wt-%

Material	C	Mn	Si	Cr	Ni	Mo	N	Nb	Ti	Cu	V	Co	Fe
Alloy 2205 (UNS S31803)	0·03	1·6	0·5	22	5·5	3·0	0·14	0·03	0·05	0·0	0·06	0·07	67·02
Alloy 255 (UNS S32550)	0·04	1·0	0·5	25	5·5	2·5	0·18	0·03	0·05	2·0	0·06	0·07	63·07



a C; *b* Mn; *c* Si; *d* Cr; *e* Ni; *f* Mo; *g* N; *h* Nb; *i* Ti; *j* Cu; *k* V; *l* Co

3 Predicted FN for alloy 255 duplex stainless steel weld with different concentrations of element (concentration of other elements held constant except for Fe, which was adjusted to compensate for the concentration varying element)

greater than 0·05% stabilises ferrite in alloy 2205, in agreement with Kotecki,[3] who also reported this. At higher concentrations of Ti, large error bars imply that more experiments are necessary. Co acts as a ferrite stabiliser at Co contents <0·2 wt-% and as a weak austenite stabiliser at higher Co contents, while Mn and Cu are not found to influence the FN value in alloy 2205.

Figure 3 shows the influence of variation in concentration of individual alloying elements on the FN value for 12 input elements in alloy 255 duplex stainless steel. It is found that Ni, N, Mn, Cu, Si, and Nb act as an austenite stabiliser for alloy 255. The observation that Mn and Cu act as austenite stabilisers in alloy 255 is different from the observation that these elements do not influence the FN in alloy 2205. Thus, depending on the base alloy composition, the role of the alloying elements varies. Similar observations were reported by Vitek *et al.*[12] The role of Ni, N, Mn, and Cu as austenite stabilisers is in agreement with reports by Kotecki.[3] The role of Si and Nb as an austenite stabiliser in alloy 255 is reported here for the first time. At low concentrations of 0·03%, Nb is not effective in forming carbides and nitrides and Nb can be ferrite stabiliser only by removing the carbon and nitrogen from austenite. Figure 3 also shows that Cr, Mo, V, and Co act as ferrite stabilisers, while Ti is observed to have a varying effect on the FN value. As in alloy 2205, in alloy 255 too Ti acts as an austenite stabilizer at low Ti content <0·05 wt-% but as a strong ferrite stabilizer at Ti contents >0·05 wt-%.

Conclusions

1. Using this generalised BNN model, the influence of variation in weld composition on the FN value has been quantified for alloy 2205 and alloy 255 duplex stainless steels.

2. The role of alloying elements Ni, Cr, N, Mo, Mn, Cu, V, and Co in influencing the FN value in duplex stainless steel welds as identified by this BNN model, is in agreement with that reported in the literature.

3. The role of alloying elements Si (as an austenite stabiliser) and Ti (as a ferrite stabiliser) in influencing the FN value in duplex stainless steel welds has been clearly demonstrated by this BNN model, while these elements are not considered in the WRC-1992 diagram.

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