

Improved Ferrite Number Prediction in Stainless Steel Arc Welds Using Artificial Neural Networks — Part 2: Neural Network Results

A new neural network model predicts Ferrite Number with significantly more accuracy than existing constitution diagrams

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ABSTRACT. The development of a neural network model, named FNN-1999, for predicting Ferrite Number in arc welds as a function of alloy composition is described in Part 1. In this paper, the results of the model are compared to other means of predicting Ferrite Number in stainless steel welds. It was found the accuracy of the FNN-1999 model in predicting Ferrite Number is superior to that of the WRC-1992 diagram, the Function Fit model and a preliminary neural network model developed earlier. The error in fitting the current model to the training set was 40% less than that for the WRC-1992 diagram. In addition, the FNN-1999 model removes the restriction found in WRC-1992 and many other constitution diagrams that each element's contribution to the Ferrite Number is constant, regardless of the overall composition. Examples are given that show that with this added flexibility of the FNN-1999 model, the impact of alloying additions varies as a function of concentration, and in some cases the variation can be quite significant.

Introduction

The ability to predict the ferrite content in stainless steel arc welds is essential, as described in detail in Part 1 (Ref. 1). Although currently available constitution diagrams are reasonably accurate in predicting Ferrite Number, improved accuracy and flexibility that takes the alloy composition into account is desir-

able (Ref. 1). Neural network models are ideally suited for predicting Ferrite Number in welds because of their flexibility and their ability to account for nonlinear behavior. In Part 1 of this paper (Ref. 1), the development of a neural network model (FNN-1999) for predicting Ferrite Number is described in detail, including the basic principles behind neural networks, the identification of the optimum network architecture and the specifications of the network weights for a "best" network for ferrite prediction. Here, in Part 2, the neural network model results are presented, including an assessment of the prediction accuracy compared with other available methods. Calculations are also presented that show composition-dependent effects of various elements and the ability of the neural network model to capture these effects when making ferrite predictions.

Optimum Neural Network Model

An optimum neural network architecture was identified in Part 1 and is shown in Fig. 1. The network consists of thirteen

input nodes, corresponding to the compositions of thirteen alloying elements (C, Cr, Ni, Mo, N, Mn, Si, Fe, Cu, Ti, Nb, V and Co), six hidden nodes and one output node (Ferrite Number). The network was trained on the same extensive data set (Refs. 2–4) ("complete training data set") used to establish the WRC-1992 constitution diagram (Ref. 5). Details regarding the development of the network are provided in Part 1 (Ref. 1). The best network is defined by a series of coefficients (weights) that correspond to the node connections in Fig. 1 (these are also given in Part 1). The range of alloying element concentrations over which the network is applied is given in Table 1. As described in detail in Part 1, non-zero concentrations must be used for eight of the elements (C, Cr, Ni, Mo, N, Mn, Si, Fe). For the remaining five elements (Cu, Ti, Nb, V, Co), a zero concentration is appropriate when chemical analysis results are not available. Some results are also presented that consider another data set (Refs. 6, 7) ("supplemental data set"). These data were not used in the training of any of the predictive models and therefore this data set represents an independent set of experimental results useful for evaluating the prediction accuracy, although the composition range it covers is more limited than the training data set (Table 1).

Results and Discussion

Prediction Comparisons of Various Models

Ferrite Number (FN) was calculated using the neural network for all alloy compositions in the data set used for training the neural network, and the predicted FN values are plotted against ex-

KEY WORDS

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Constitution Diagram
Neural Network
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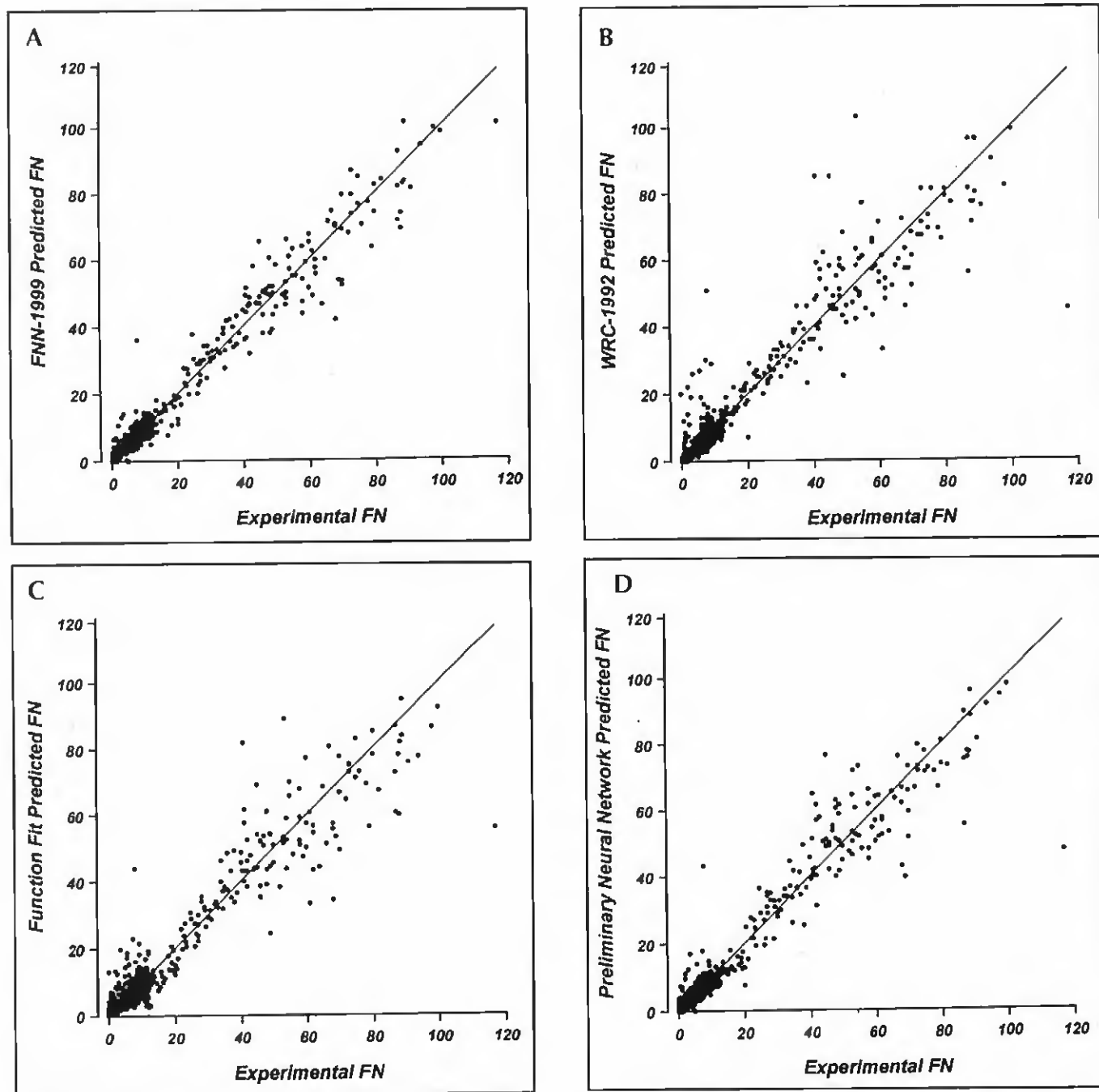


Fig. 2 — Experimentally measured FN vs. predicted FN for the complete training data set for four different predictive models. A — FNN-1999 model from the present study; B — WRC-1992 constitution diagram (Ref. 5); C — Function Fit model (Ref. 8); D — earlier neural network model that considered only eight elements (Ref. 9).

The root mean square (RMS) errors between the measured and predicted FN values for all four FN prediction methods are compared in Table 3. These errors provide a quantitative measure of the degree to which the various models "fit" the complete data set on which they were all trained. While the Function Fit model and WRC-1992 diagram accuracies are comparable, the earlier eight-element neural network model showed a significantly reduced RMS error. The present

neural network model, FNN-1999, with the extension from 8 to 13 elements, has the lowest RMS error of all four models, with a 40% improvement over the WRC-1992 constitution diagram RMS error and a 27% improvement over the earlier neural network model.

When comparing the FNN-1999 model for Ferrite Number prediction with the WRC-1992 diagram, it should be noted the WRC-1992 diagram has a quoted upper limit for the nickel equiva-

lent (Ni_{eq}) of 17. This limit was imposed due to the scarcity of data for $Ni_{eq} > 17$, but Lake (Ref. 11) has recently shown the WRC-1992 diagram is accurate beyond this limit. No attempt was made in the present study to exclude the experimental data with $Ni_{eq} > 17$ in the training routine. In the entire experimental data set of 961 points, there were 89 measurements on alloy compositions with $Ni_{eq} > 17$. The RMS error of the WRC-1992 predictions for these 89 measurements was cal-

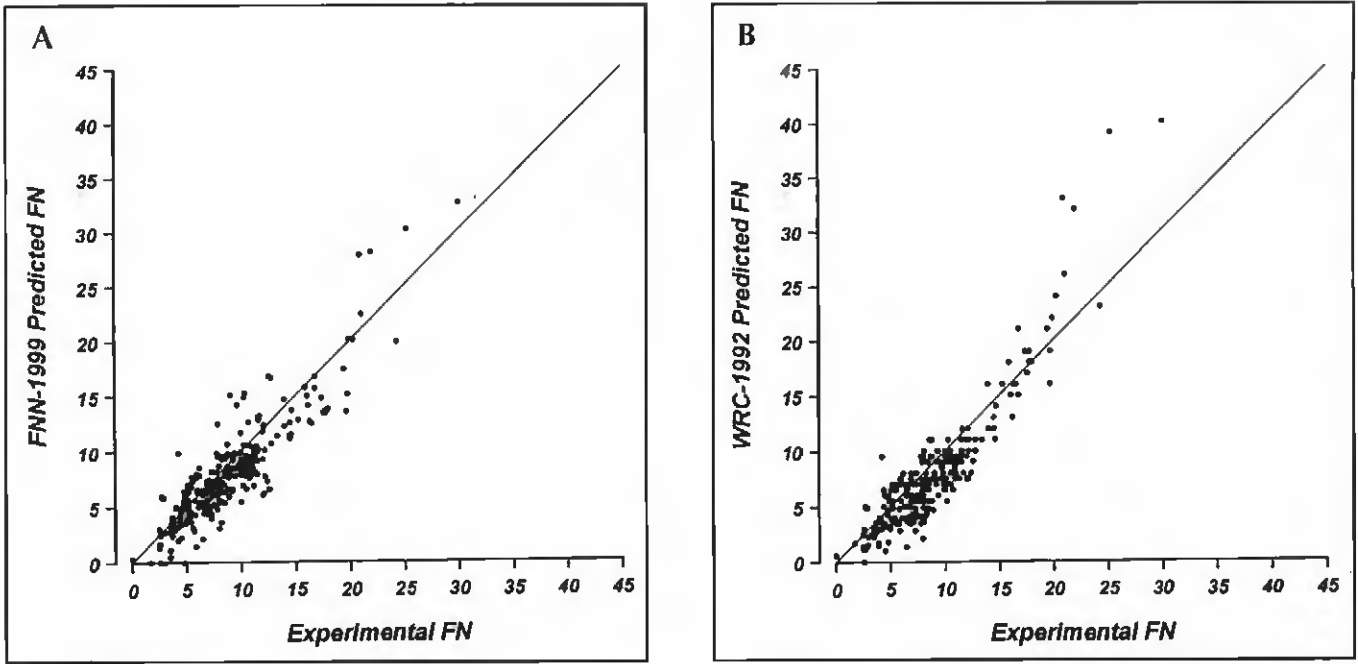


Fig. 4 — Experimentally measured FN vs. predicted FN for the supplemental data set for two different predictive models. A — FNN-1999 model from the present study; B — WRC-1992 constitution diagram (Ref. 5).

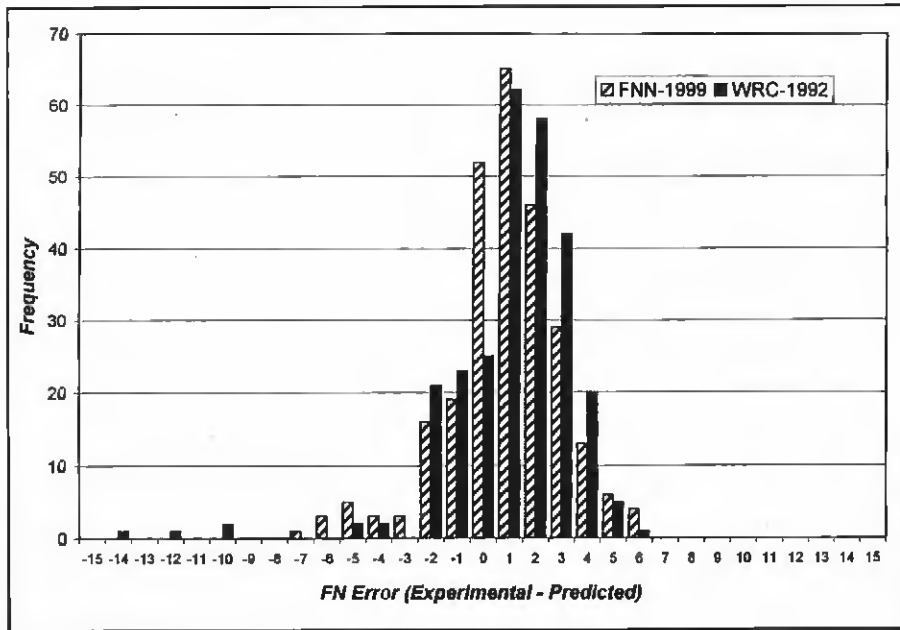


Fig. 5 — Error distribution (experimental FN; predicted FN) for the supplemental data set for the FNN-1999 model and the WRC-1992 constitution diagram (Ref. 5).

Table 5 — Comparison of Root Mean Square Errors for Supplemental Data Set for Four FN Prediction Methods

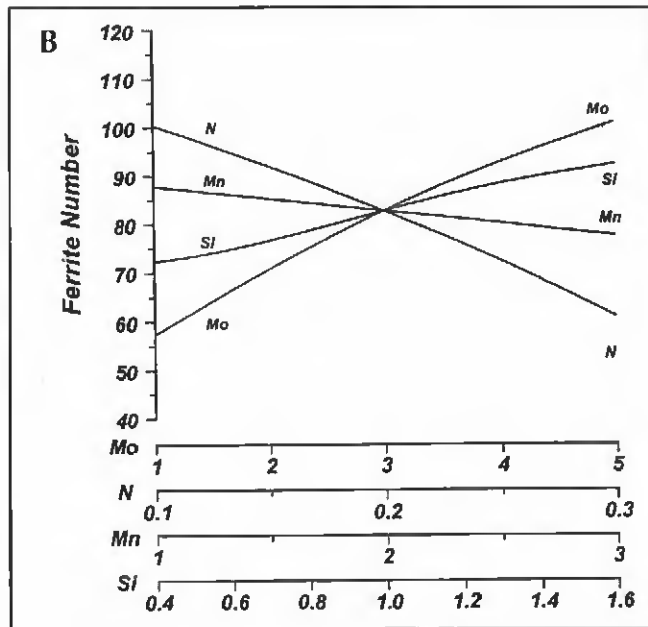
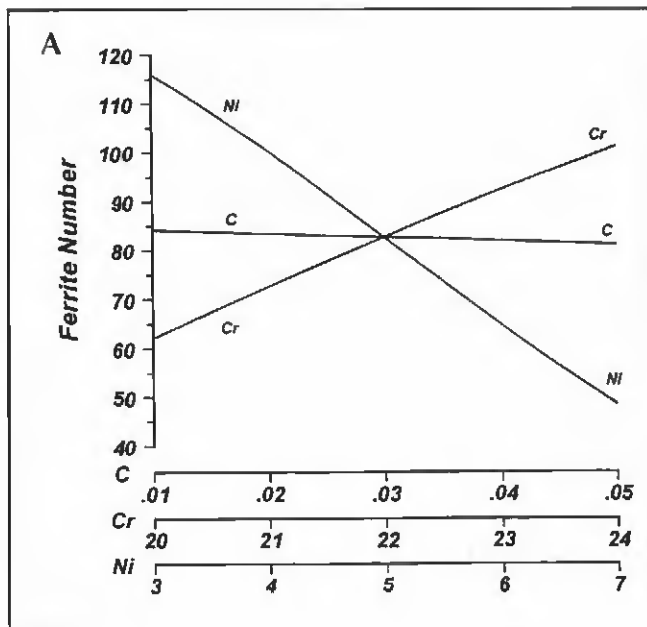
Prediction Method	Root Mean Square Error
FNN-1999 Model	2.3
WRC-1992 (Ref. 5)	2.6
Function Fit Model (Ref. 8)	5.1
Earlier Neural Network Model (Ref. 9)	2.6

Predictability Evaluation of the FNN-1999

The final method for evaluating the predictability of the neural network was to train the network on an “almost complete” training set, and then test the network on the few data points (~ 1%) left out of the training set. This was done for ten different 99%-1% combinations. This method provides a better indication of the prediction RMS error than that shown in Table 3 since the predictions are for new alloy compositions not used during the training of the network. The RMS errors in Table 3 are an indication of how well the neural network model (or the other models) can be fitted to the data, while the RMS error from the 99%-1% calculations is a true prediction error for the 1% test data that are not used during the network training. The average RMS error for these ten tests was 3.3. This value is comparable to the 3.5 RMS error

set covered a relatively small range in FN. Of the 265 data points, 254 corresponded to FN ≤ 18. This is the range over which the WRC-1992 diagram was optimized. Therefore, the fact that the FNN-1999

model is more accurate than the WRC-1992 diagram, even in this limited range of FN, is significant, even though the extent of improvement is less than that for the training data set (compare Tables 3 and 5).



ered, comparable to a typical austenitic stainless steel, was (in wt-%) 65.9 Fe-20 Cr-11 Ni-0.08 C-0.01 Mo-0.01 N-2 Mn-1 Si. The FN was calculated using the FNN-1999 model for this base composition as well as for a range of concentrations for each of 12 elements (Fe was not considered since it was varied to compensate for the independently varying concentration). The range of values that were examined is listed in Table 6. The calculated FN vs. concentration is plotted in Fig. 6. Note the concentration scale varies according to the element, and only one element concentration is allowed to change at a time, with all other elements (except Fe) held constant at the base metal concentration.

Several features are immediately noticeable in Fig. 6. First, the effect of concentration on FN varies dramatically according to the element that is varied, with some elements increasing the FN as the concentration increases and others showing the opposite effect. It is also clear the change in FN is not necessarily linear with concentration. In particular, a nonlinear variation is found for V and Si, and, to a lesser degree, for Ni and Ti. For the austenitic stainless steel base composition, several elements produce a positive slope for the curves, including Cr, Ti, Mo, Nb and Cu. The elements that result in a negative slope are Ni, V, C, N, Mn and Co. The slope of the FN vs. concentration curve changes from positive to negative for Si. The identification of these trends is extremely valuable, and is totally overlooked by currently available constitution diagrams. The grouping of elements according to the slopes corresponds to the process of grouping elements in the Cr_{eq} and Ni_{eq} expressions.

Various expressions for the Cr_{eq} and Ni_{eq} are available (Refs. 5, 12). In general, some or all of the following elements are included in the Cr_{eq} expressions: Cr, Ti, Mo, Nb, V and Si. Similarly, some or all of the following elements are included in the expressions for the Ni_{eq} : Ni, C, N, Mn, Co and Cu. In most cases, the elemental groupings found by the FNN-1999 model are identical to the groupings that have been suggested in the literature over the years. The few exceptions are Si, Cu and V, which are discussed below.

The neural network calculations indicate that Si changes from a ferrite stabilizer to a weak austenite stabilizer at higher concentrations. When included in traditional constitution diagrams, Si is treated as a ferrite stabilizer. The reversal in behavior indicated by the FNN-1999 model and shown in Fig. 6 may explain the difficulty in identifying a statistically significant coefficient for Si in the WRC-1988 diagram (Ref. 13), the predecessor to the WRC-1992 diagram. As a result, Si was excluded from both of these diagrams.

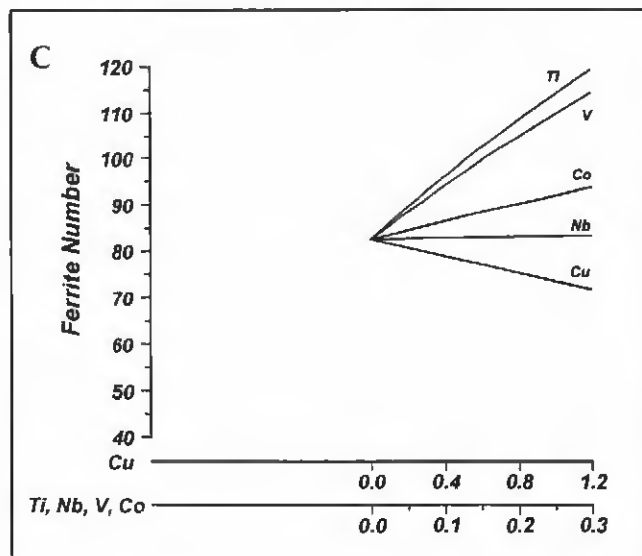


Fig. 7 — Calculated FN vs. concentration for a typical duplex stainless steel base composition. Calculations were performed using the FNN-1999 model. A — C, Cr, Ni; B — Mo, N, Mn, Si; C — Cu, Ti, Nb, V, Co. The base metal concentration is 66.77 Fe-22 Cr-5 Ni-3 Mo-2 Mn-1 Si-0.03 C-0.2 N. The plots show the variation in FN when one element is varied and all other concentrations are held constant at the base metal value (except Fe, which is adjusted to compensate for the varying element concentration).

Figure 6 indicates Cu is a very weak ferrite stabilizer for the austenitic stainless steel base composition. This is opposite to its role as an austenite stabilizer as identified in the WRC-1992 diagram. However, it should be noted the magnitude of the effect of Cu for the austenitic stainless steel base composition, as calculated by the FNN-1999 model, is very small. A change in Cu content from 0 to 0.6 results in an increase in FN of only 0.5, which is negligible. As shown later, for a different,

tration of only one element was varied (with the Fe concentration adjusted accordingly), all other element concentrations were held constant at the base metal value. The effect of concentration on FN for several elements is quite different from the behavior shown in Fig. 6. The effect of V is the opposite of what was seen before; V changes from a weak austenite stabilizer to a very strong ferrite stabilizer. Just the opposite holds for Cu; it changes from a weak ferrite stabilizer for an austenitic stainless steel base composition to an austenite stabilizer for a duplex steel base composition. The latter behavior is the same as indicated in the WRC-1992 diagram. Increasing Si concentration leads to a steady increase in FN, without the reversal seen in Fig. 6.

The slopes in Fig. 7 as well as the normalized values (with respect to the Cr or Ni slopes) are listed in Table 9. It is interesting to compare the potency of Cr and Ni for the two base compositions. Examination of the average slopes for these two elements in Tables 7 and 9 shows that Cr is a stronger ferrite stabilizer (steeper slope) and Ni is a stronger austenite stabilizer for the duplex stainless steel base composition. The values of the normalized slopes in Table 9 are also very different from those in Table 7 for many elements. This is a direct indication of a change in behavior when the base composition is changed from that of an austenitic stainless steel alloy to a duplex steel. The effect of C is diminished considerably. On the other hand, the influence of Ti and Co is enhanced. The effects of Mo, Nb and Mn are relatively unchanged.

Additional Comments

The use of neural networks for predicting Ferrite Number has an additional, potentially important advantage in that, in theory, process variables can be included as well as composition as inputs to the model. For example, many studies have shown that at high cooling rates prevalent during laser beam or electron beam welding, the residual ferrite content can be significantly different than that found for the same alloy under typical arc welding conditions (Refs. 15–21). The dramatic changes in ferrite content are often attributable to a change in the solidification mode so that an alloy that solidifies in the primary ferrite mode under near-equilibrium conditions can change to primary austenite solidification when rapidly cooled. In addition, rapid cooling after solidification will affect the solid-state transformation kinetics. In theory, this additional factor that influences Ferrite Number can be incor-

porated into a neural network model. Such an enhancement is planned for future work. Furthermore, if the training data set included data on the specific arc welding technique, in addition to the information on composition and FN, then the effect of arc welding process on the final FN could be included as well. This was not done in the present case since this additional information on arc welding process was not available.

The FNN-1999 model cannot be condensed into a simple pictorial form such as the WRC-1992 diagram. However, as shown in Figs. 6 and 7, important information on the influence of individual elements on the FN can be readily calculated. The neural network is especially easy to use in these types of calculations since the entire neural network can be easily converted into a spread sheet format. These types of calculations can yield even more useful information than the pictorial constitution diagram since the changing influence of various elements can be identified directly. For the interested reader, the FNN-1999 model is available over the Internet and sample calculations can be made. The neural network can be accessed at the following Web site: <http://engm01.ms.ornl.gov>.

Finally, it is interesting to speculate on other potential applications of neural network models beyond simply Ferrite Number prediction. In many cases, Ferrite Number prediction is not an end in itself. Ultimately, Ferrite Number prediction is a means for estimating an alloy's susceptibility to weld cracking or its mechanical properties, including its corrosion resistance. In this regard, it may be possible to use neural networks to directly correlate composition with these properties and bypass the intermediate Ferrite Number stage completely. Neural networks are ideally suited for such applications. Several neural network models have already been developed to predict weld alloy properties (Refs. 22, 23). The largest impediment for using neural network models to predict properties of stainless steels directly is the availability of a sufficiently complete database. If such a database were available, development of the required neural network models could easily follow and the need for constitution diagrams and Ferrite Number prediction could be eliminated altogether.

Conclusions

A neural network model, identified as FNN-1999, was developed to relate residual ferrite content in arc welds to alloy composition. Details of the neural network development are presented in

Part I. The model uses the concentrations of thirteen elements (C, Cr, Ni, Mo, N, Mn, Si, Fe, Cu, Ti, Nb, V and Co) and shows a significant improvement in FN prediction accuracy compared to an earlier neural network model that considered the concentrations of only eight elements. It is also shown that the fitting error for the FNN-1999 model is 40% less than that for the WRC-1992 constitution diagram. In addition, the FNN-1999 model has the ability to account for significant variations in the influence of individual alloying additions as a function of overall alloy concentration. It is shown that such variations in the effect of alloying additions can be significant. For some alloying additions, the basic nature of their influence, in terms of the element behaving as an austenite stabilizer or ferrite stabilizer, was found to be reversed when the base composition was changed. The new FNN-1999 model provides a simple and quick means for predicting Ferrite Number in arc welds with a substantial improvement in the accuracy of the prediction compared to other models that are currently available.

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References

1. Vitek, J. M., Iskander, Y. S., and Oblow, E. M. 2000. Improved ferrite number prediction in stainless steel arc welds using neural networks — part 1: neural network development. *Welding Journal* 79(2): 33-s to 40-s.
2. Kotecki, D. J. 1986. Ferrite control in duplex stainless steel weld metal. *Welding Journal* 65(10): 273-s to 278-s.
3. Kotecki, D. J. 1989. Heat treatment of duplex stainless steel weld metal. *Welding Journal* 68(11): 431-s to 441-s.
4. McCowan, C. N., Siewert, T. A., and Olson, D. L. 1989. Stainless steel weld metal: prediction of ferrite content. *WRC Bulletin* 342: 1–36.

