Prediction of Jominy Hardness Profiles of Steels Using Artificial Neural Networks

W.G. Vermeulen, P.J. van der Wolk, A.P. de Weijer, and S. van der Zwaag

Jominy hardness profiles of steels were predicted from chemical composition and austenitizing temperature using an artificial neural network. The neural network was trained using some 4000 examples, covering a wide range of steel compositions. The performance of the neural network is examined as a function of the network architecture, the number of alloying elements, and the number of data sets used for training. A well-trained network predicts the Jominy hardness profile with an average error of about 2 HRC. Special attention was devoted to the effect of boron on hardenability. A network trained using data only from boron steels produced results similar to those of a network trained using all data available. The accuracy of the predictions of the model is compared with that of an analytical model for hardenability and with that of a partial least-squares model using the same set of data.

Keywords

chemical composition, hardenability, jominy end-quench test, neural networks, statistical modeling

1. Introduction

THE Jominy or end-quench test is a simple, widely used method for characterizing the hardenability of steels. This hardenability is determined entirely by the steel microstructure, which in turn is primarily determined, for the fixed range of cooling rates on the Jominy test sample, by the alloying elements. Therefore, it should be possible to predict the hardenability of a steel strictly on the basis of its chemical composition, assuming other parameters to be constant.

Previous attempts to predict hardenability failed to develop an accurate empirical model over a wide range of steel grades because of use of a predefined functional relationship between the hardness profile and the chemical composition of a steel. These predefined relations were generally assumed to be linear, which is not always the case. Neural networks are more suitable to model the effect of chemical composition on hardenability because they require no prior assumptions concerning the functional dependence. Furthermore, neural networks can readily handle nonlinear dependencies.

This paper describes the development of a neural network to predict the Jominy hardness profile of steels based on chemical composition and austenitizing temperature. A large data set containing the chemical compositions, austenitizing temperatures, and Jominy hardness profiles of some 4000 low-alloy and boron-containing steels was supplied by Nedstaal BV. The influence of the number of hidden nodes—the architecture of the neural network—and of the number of training data on network performance is investigated. Also, the performance of the neural network models is compared with that of an empirical model and of a linear partial least-squares model.

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2. The Jominy or End-Quench Test

The Jominy or end-quench test (Ref 1) is a robust test that is widely used to characterize the hardenability of steels. In this test, a specimen with a diameter of 1 in. and a length of 3 or 4 in. is austenitized for approximately 30 to 35 min. The austenitizing temperature depends on the composition of the steel being investigated. After this heat treatment, one end of the specimen is quench hardened for at least 10 min in a water stream with a temperature of 5 to 30 °C; the other end is cooled in air.

As a result, a cooling-rate gradient develops over the length of the specimen, with the highest cooling rate at the quenched end. This gradient results in different microstructures—and thus different hardnesses—along the length of the specimen. The hardenability of the steel is expressed by measuring the hardness of the specimen on the Rockwell C scale at intervals of $1/16$ in., beginning at the quenched end. These Jominy hardness profiles characterize the hardenability of a steel.

3. Neural Networks

Statistical techniques may provide a useful alternative for any process that cannot be described with sufficient accuracy using physicomathematical models. In situations where tradi-

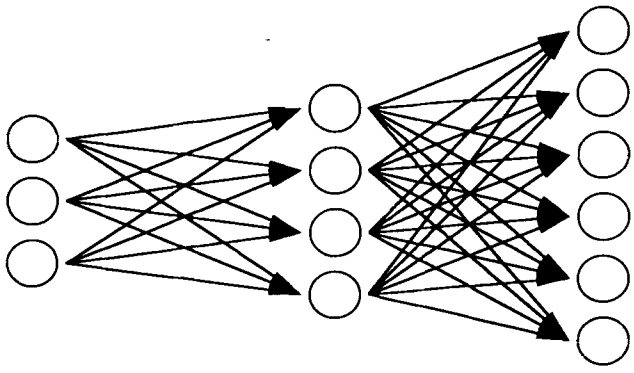

Fig. 1 Schematic representation of a hierarchical neural network. Data are transferred from left to right along the arrows; the circles represent the nodes or neurons.

tional statistical techniques fail to provide an accurate model, as in the case of strong nonlinearity, a new statistical technique called neural network modeling may be successful. There are many types of neural networks. This study used a feed-forward, hierarchical neural network—feed-forward, because the information is processed in one direction, from input to output; hierarchical, because the processing elements are ordered in layers. This type of network is usually employed for modeling. Neural networks are described in detail in Ref 2 to 4.

A feed-forward, hierarchical neural network is shown schematically in Fig. 1. The basic unit in a neural network is its processing element, called a node or a neuron. In hierarchical neural networks, these nodes are ordered in layers. The network used contains three layers: an input layer, a so-called hidden layer, and an output layer. Each node in a layer is connected, via a weight factor, with each node in the preceding layer, so the neural network is fully connected. The number of nodes in the input layer equals the number of input parameters. The number of nodes in the output layer equals the number of output parameters. The optimum number of nodes in the hidden layer depends on the complexity of the problem.

Each node computes the inner product of its input values and their weight factors and passes this value to a sigmoid transfer function, which produces the output signal. To determine these weight factors, the network must be trained. Our neural network was trained using supervised training with back-propagation of error as the training rule. For a detailed description of network training procedures, see Ref 5.

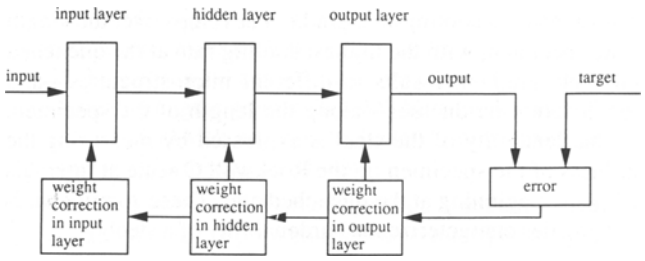

Fig. 2 Flowchart of the training cycle in a feed-forward, hierarchical neural network

The training cycle is outlined in Fig. 2. To start, random values are attributed to the weight factors. Then, the input data of one sample are processed by the network, and the output is compared with the target output. The difference between these values—the error in prediction—is a measure for the weight factor adaption. This adaption takes place in the reverse direction, known as back-propagation of error. First, the weight factors of the output nodes are adapted, then the weight factors of the nodes in the hidden layer, and then those of the input layer. Once the weight factors have been adapted for all samples, the training cycle is repeated until the differences between calculated and target output values are minimized sufficiently.

At large numbers of training cycles, the network starts to model not only the functional dependencies between input and output parameters but also the noise in the data set. This is called overtraining. To prevent the network from overtraining, the data are split into a relatively large training set and a smaller test set. The weight factors in the network are adjusted using the data in the training set only. In case of overtraining, the error for the training set decreases while that for the test set increases with further training. At this point, training is stopped.

Once the network is trained, the weight factors are fixed and the neural network may be used to calculate the output for an arbitrary set of input data. A major advantage of the neural network models is the ability to vary just one parameter, while keeping the remaining parameters constant at selected values. Such information cannot always be obtained otherwise.

4. Data Handling

Prior to training of the first network, some data handling was applied. First, the appropriate input and output parameters for the network were selected. The concentrations of 16 chemical elements and the austenitizing temperature were available as potential input parameters. The ten most relevant elements

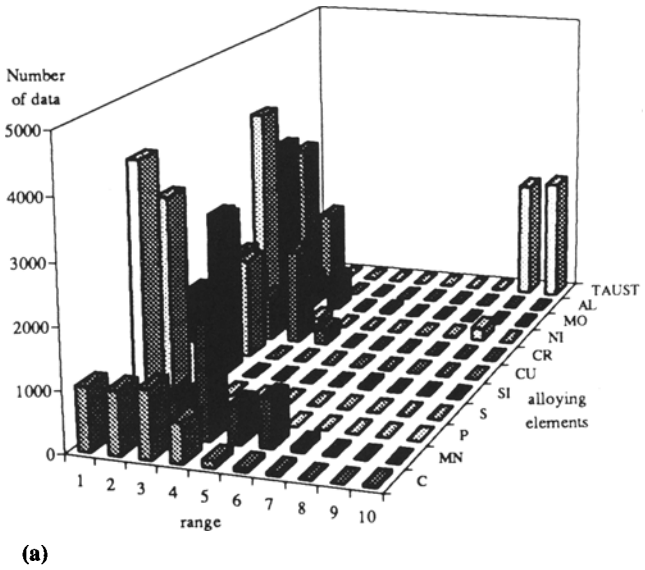

Fig. 3 Distribution of data before (a) and after (b) data selection

were selected. To approach the ideal situation of a uniform distribution of the data over the range of concentrations, some 75 steels with anomalous compositions were excluded. A data set of 3874 steel compositions with corresponding Jominy hardness profiles remained. The distribution of the data before and after data selection is shown in Fig. 3.

The input parameters for this network, referred to here as network 1, were ten alloying element concentrations and the austenitizing temperature, which ranged from 840 to 960 °C. The concentration ranges of the elements were:

Element	Concentration, wt %
Carbon	0.09-1.04
Manganese	0.35-1.54
Phosphorus	0-0.24
Sulfur	0-0.23
Silicon	0.01-0.34
Copper	0.01-1.26
Chromium	0-1.67
Nickel	0.01-1.7
Molybdenum	0-0.45
Aluminum	0-0.066

The output consisted of the hardness values at 19 intervals of $1/16$ in. from the quenched end (J1 to J19). In some cases, the Jominy hardness profiles were not completely characterized. The hardness values at the positions relatively far away from the quenched end had not been measured. In these cases, missing hardness values were assumed to be equal to the hardness value at the highest Jominy position measured. No quantitative grain size information was available, but all steels were known to be fine grained. Of the total data set, 75% was used for training and 25% was used for validation.

5. Results and Discussion

5.1 *Influence of Number of Nodes in the Hidden Layer on Network Performanc*

Four measured and predicted Jominy hardness profiles are shown in Fig. 4 to illustrate the predictive capabilities of network 1 over a wide range of steel grades. The chemical compositions and austenitizing temperatures of these four steels are shown in Table 1. In this case, the network was trained using 15 nodes in the hidden layer. Clearly, network 1 predicts the four different Jominy profiles with high accuracy.

Figure 5 shows the influence of the number of nodes in the hidden layer—the network architecture—on network performance. The error plotted is the product of the range of hardness variations at that particular Jominy position and its relative standard deviation (RSD), which is defined as:

$$\text{RSD} = \sqrt{\frac{\sum_{\text{all samples}} (\text{Measured} - \text{Predicted})^2}{\text{Number of samples} - 1}}$$

The error decreases with an increasing number of nodes in the hidden layer. The error in hardness for Jominy positions 3 to 8 is always higher than for the other Jominy positions. This behavior can be explained as follows: The hardnesses near the edge of the specimen are almost completely determined by carbon content (Ref 6) and vary little with position. At high Jominy positions, little variation in the cooling rate occurs; hence, hardness varies little with position. In the intermediate zone, however, hardness varies strongly with position. A little variation or error in Jominy distance results in a high variation of hardness, and thus in a high experimental error in this region.

For the complete Jominy hardness profile, the difference between the predicted and the experimental value is of the same magnitude as the experimental error. Of course, errors in element concentration also contribute to the difference between predicted and expected values. It should be pointed out that no signs of overtraining of the network, which would also increase the error in the predictions for the test set, were observed.

As it turned out, neither the elements phosphorus, sulfur, and copper nor the austenitizing temperature appeared to significantly influence the Jominy hardness profile. Therefore, these elements and the austenitizing temperature were omitted as input parameters in subsequent networks. The austenitizing temperature had been chosen on the basis of carbon content, so these two input parameters are highly correlated. Highly correlated parameters offer no extra information, so one of them can be omitted.

Furthermore, it was found that the prediction of hardness values for high-carbon steels (C > 0.65%) by network 1 was not accurate. We believe that the reason for this deviant prediction can be found in the inequality of the data distribution. Only some 50 steels in the data set had a carbon content higher than 0.65%, so the majority of the steels—almost 3800 sets—had a carbon content in the 0.09 to 0.65% domain. The network did not seem to recognize the variations caused by the high carbon content as significant, but saw them merely as noise.

A new network (network 2) was trained with nine alloying elements as input parameters: carbon, manganese, silicon, chromium, nickel, molybdenum, and aluminum, plus new elements boron and nitrogen. The output parameters remained unchanged. The number of nodes in the hidden layer was fixed at 15, because network 1 yielded the best prediction for this number of hidden nodes. The concentration ranges of the elements used as input parameters for network 2 were:

Element	Concentration, wt %
Carbon	0.09-0.65
Manganese	0.35-1.54
Silicon	0.01-0.34
Chromium	0-1.67
Nickel	0.01-1.7
Molybdenum	0-0.45
Boron	0-0.0057
Aluminum	0-0.066
Nitrogen	0-0.014

Figure 6 shows the errors in prediction for test and training sets as a function of Jominy distance. Again, the difference between predicted and measured values is of the same magnitude as the experimental error of the hardness value itself. However, it is concluded that the overall performance of the network 2 is better than the performance of network 1 because it is more compact, having fewer input parameters.

5.2 *Influence of Number of Data Sets on Network Performance*

Section 5.1 showed that an artificial neural network with 15 hidden nodes can predict the hardenability of steels from their chemical composition using some 2900 (75% of 3900) data sets for training. However, the minimum number of data sets required to train an accurate network is yet unknown. Therefore, several 9-15-19 networks were trained with different numbers of data sets. The compositional ranges defined in the previous section were covered in all training cycles. The prediction errors for these networks are shown in Fig. 7, which demonstrates that 800 sets of data are sufficient to build a satisfactory model. All networks were validated with an identical test set containing 667 data sets.

Clearly, the number of training data sets required depends on both the number of input parameters and the nonlinearity of the functional dependence. Generally, the number of data sets should be between 2^N and 3^N, where N is the number of independent orthogonal input parameters.

5.3 *Influence of Boron Concentration on Prediction of Jominy Hardness Profiles*

Boron holds a special place among the steel alloying elements because of its significant effect on hardness even at very low concentrations. The presence of boron in sizable amounts influences steel hardenability in two ways (Ref 7). First, the incubation time for ferrite formation is increased, and the nucleation rate after the incubation period is lowered by the formation of borocarbides along the austenite grain boundary. Second, many undissolved borocarbides are distributed homogeneously in the austenite grains without any specific crystallographic relationship with the austenite lattice. They provide nucleation sites during subsequent cooling, resulting in a finer structure and thus a higher hardness.

However, at higher carbon concentrations (C > 0.25%), excessive borocarbide formation makes boron less effective in reducing the rate of ferrite formation, resulting in an optimum boron concentration for maximum hardenability (Ref 7). This optimum boron concentration is on the order of 15 to 20 ppm, but its exact value is still debated.

Figure 8 shows the influence of boron concentration on the predicted Jominy hardness profiles for two steels with different carbon concentrations. These results were obtained using network 2. The chemical compositions of these two steels are given in Table 2. According to network 2, the hardnesses at Jominy distances 2 to 8 are most influenced by boron concentration. It appears that at boron concentrations greater than 0.002%, additional boron has little effect on hardness at these Jominy distances. At greater Jominy distances, the influence of

Table 1 Chemical compositions and austenitizing temperatures of the steels in Fig. 4

Steel No.	Austenitizing temperature, °C	Composition, wt %									
		C	Mn	P	S	Si	Cu	Cr	Ni	Mo	Al
1	920	0.13	0.67	0.013	0.014	0.06	0.19	1.04	0.07	0.23	0.037
2	860	0.48	0.67	0.007	0.013	0.21	0.08	1.02	0.47	0.92	0.041
3	820	0.60	0.61	0.012	0.022	0.24	0.08	0.06	0.05	0.01	0.020
4	860	0.51	0.83	0.008	0.015	0.23	0.12	0.50	0.56	0.18	0.025

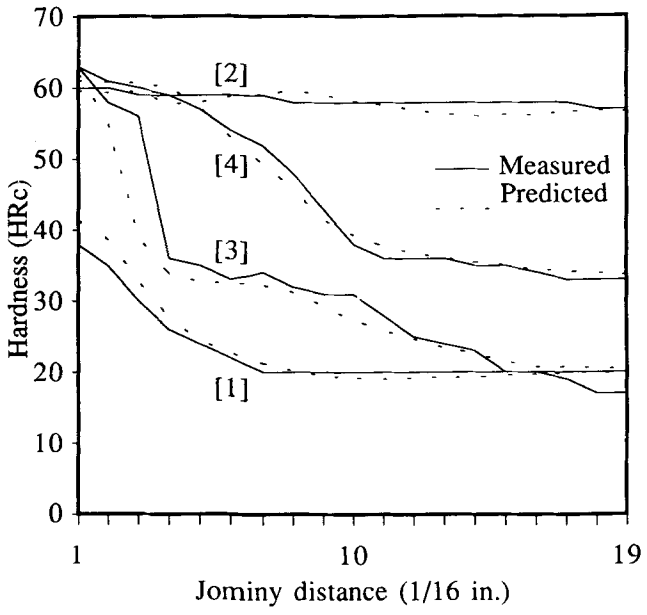

Fig. 4 Four different experimental and predicted Jominy hardness profiles

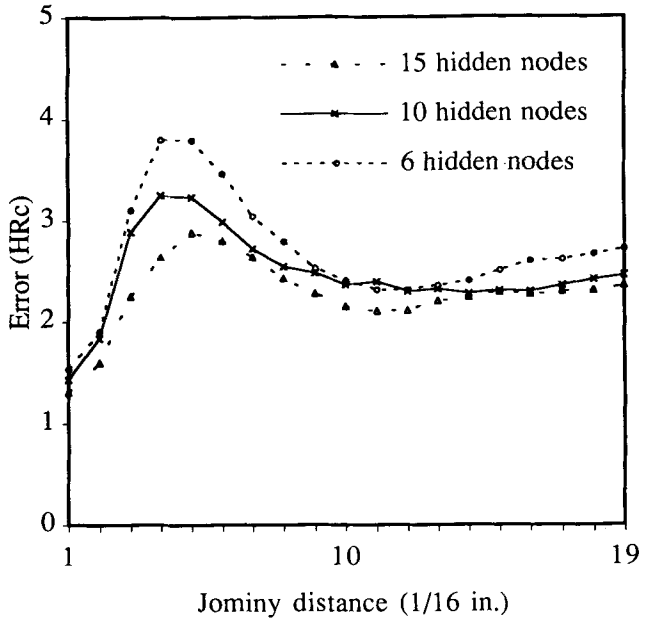

Fig. 5 Influence of number of hidden nodes on prediction error of network 1

boron is small. Furthermore, the trend is reversed: Higher boron concentrations result in lower hardness values.

To examine the influence of boron on hardenability in more detail, a special network was trained specifically for boron-containing steels. These steels were selected from the initial set of data. Only some 1100 boron-containing steels were available for training and validation of the boron network. In this case, all data were used for training. To avoid overtraining, the number of iterations was kept at the same level as for the networks trained earlier. The concentration ranges of the elements used as input parameters in the boron network were:

Element	Concentration, wt %
Carbon	0.14-0.41
Manganese	0.53-1.42
Silicon	0.01-0.3
Chromium	0-0.5
Nickel	0.02-0.13
Molybdenum	0-0.05
Boron	0.002-0.0057
Aluminum	0-0.063
Nitrogen	0-0.014

Note that the minimum boron concentration for this network was 0.002%, in contrast to network 2, where it was 0%. The boron network was trained using 15 nodes in the hidden layer.

To compare the predictions of network 2 with those of the boron network, the hardness values at the J3 and J4 positions are plotted in Fig. 9. There is a good agreement between the predictions of both networks in the overlapping concentration range. The boron network yields no reliable predictions for boron concentrations below 0.002%. The predictions of both networks do not disagree with the optimum boron concentration value reported in the literature (Ref 7). However, an optimum concentration, if present, is not well defined.

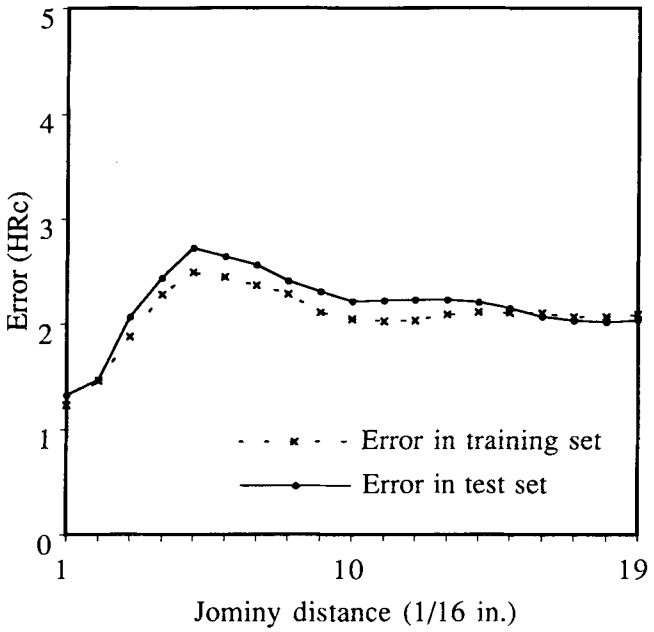

Fig. 6 Error in prediction for test and training sets of network 2

5.4 *Comparison of the Neural Network Model with the Comprehensive Model of Just*

The predictions of the neural network models were compared with those of the so-called comprehensive model of Just for the hardenability of steels (Ref 8). The Just model was used for comparison because it does not require grain size values in the input data, as do most other empirical models. The concentration ranges over which the Just model is valid are:

Element	Concentration, wt %
Carbon	0.10-0.64
Manganese	0.45-1.64
Silicon	0.15-1.78
Chromium	0.02-1.55
Nickel	0.01-1.85
Molybdenum	0-0.45
Vanadium	0-0.19

Only those steels in our original data set that fell within these ranges— some 3000—were used to determine the accuracy of the Just model. The results are shown in Fig. 10. Both neural network models outperformed Just's comprehensive model; the error of prediction of networks 1 and 2 was three to four times lower than that of the Just model. Only the first Jominy value was predicted with the same accuracy by both types of models.

Table 2 Chemical compositions of the two classes of steel plotted in Fig. 8

	Composition, wt %								
Class	C	Mn	Si	Cr	Ni	Mo	B	Al	N
1	0.39	0.65	0.22	0.22	0.07	0.02	0, 0.002, or 0.005	0.038	0.008
2	0.18	1.12	0.2	0.05	0.05	0.01	0, 0.002, or 0.005	0.035	0.011

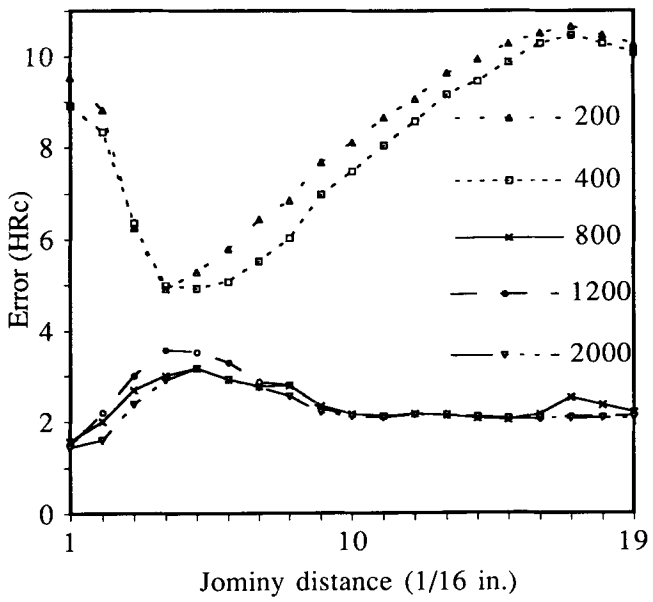

Fig. 7 Influence of number of training data sets on prediction error of network 2

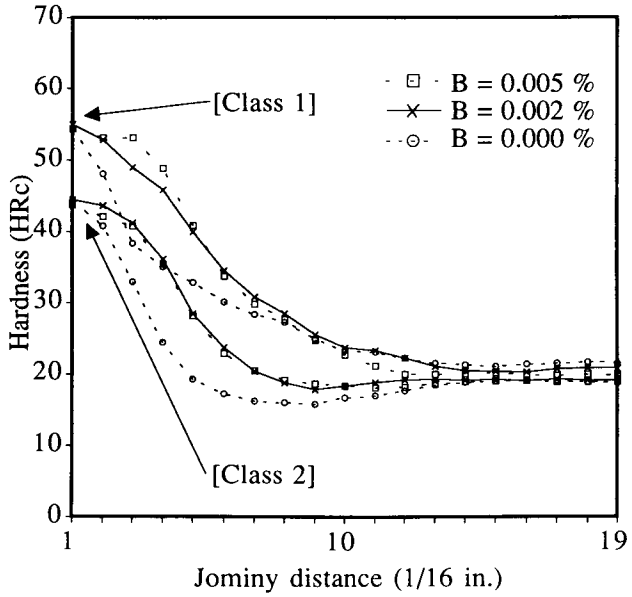

Fig. 8 Influence of boron concentration on prediction of Jominy hardness profiles for two classes of steel (see Table 2). The predictions were made by network 2.

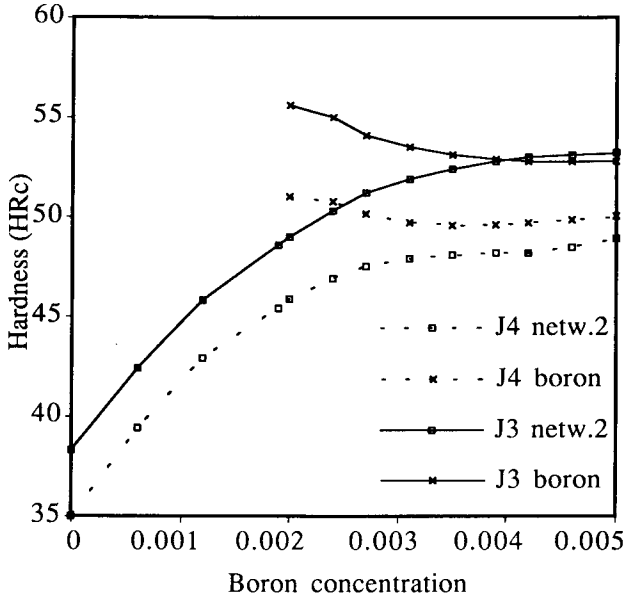

Fig. 9 Influence of boron concentration on the predicted Jominy values J3 and J4 by network 2 and by the boron network

5.5 *Comparison of the Neural Network Models with a Partial Least-Squares Model*

Partial least-squares (PLS) is a multivariate regression method based on the prediction of dependent (output) variables using only linear combinations of independent (input) variables. This is in contrast to neural networks, which allow nonlinear dependencies. The PLS method is described in detail by Geladi and Kowalski (Ref 9, 10).

The PLS method was used in the same way as the neural networks. The errors of prediction of the PLS model are also shown in Fig. 10. The neural network models had a lower error of prediction than the PLS model; only the hardness at the first Jominy position was approximated with the same accuracy. However, the PLS model was substantially more accurate than the Just model.

6. Conclusions

It is possible to predict the Jominy hardness profiles of steels from chemical composition quite accurately using feed-forward, hierarchical neural networks. The errors of prediction for the neural network models are of the same magnitude as the errors in the hardness values themselves. For the range of steel compositions investigated, approximately 800 sets of data were sufficient to build an accurate model using nine alloying element concentrations as input parameters. Special attention was devoted to the effect of boron on hardenability. The network trained using data only from boron-containing steels yielded approximately the same results as the network trained using all data sets available, indicating the robustness of the neural network models. The neural network models are much more accurate than the comprehensive model of Just and a PLS model.

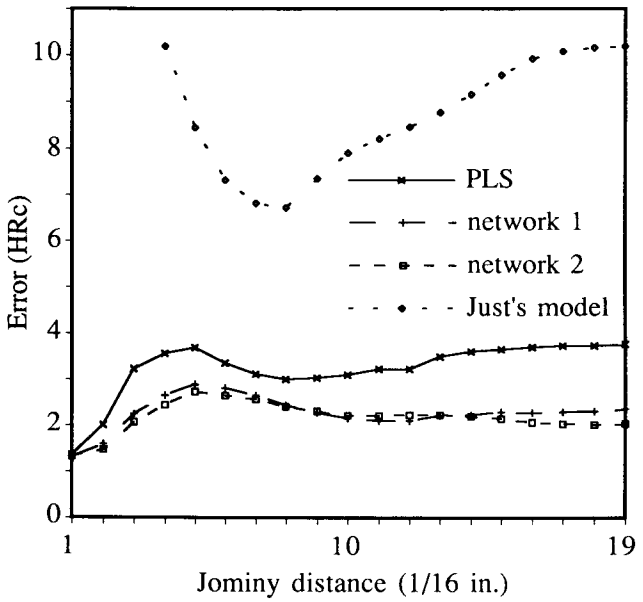

Fig. 10 Comparison of neural networks 1 and 2 with the comprehensive model of Just and a PLS model

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