Modeling medium carbon steels by usingartificial neural networks

A Project Report Submitted in partial fulfillment of the degree of

Master of Computer Application

By

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CERTIFICATE

This is to certify that the Project Report entitled "**Modeling medium carbon steels by using artificial neural networks**" submitted by **Ankit Kumar** bearing **Reg.No. 18MCMC23** and **Gujjuka Divya** bearing **Reg.No. 18MCMC48** in partial fulfillment of the requirements for the award of Master of Computer Application is a bonafide work carried out by them under my supervision and guidance.
The Project Report has not been submitted previously in part or in full to this or any other University or Institution for the award of any degree or diploma.

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DECLARATION

We, **Ankit Kumar** and **Gujjuka Divya** hereby declare that this dissertation entitled **"Modeling medium carbon steels by using artificial neural networks"** submitted by us under the guidance and supervision of **Dr. M Nagamani** is a bonafide work. We also declare that it has not been submitted previously in part or in full to this or any other University or Institution for the award of any degree or diploma.

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Ankit Kumar
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Abstract

An artificial neural network (ANN) model has been developed for the analysis and simulation of the correlation between the mechanical properties and composition and heat treatment parameters of low alloy steels. The input parameters of the model consist of alloy compositions (C, Si, Mn, S, P, Ni, Cr, Mo, Ti, and Ni) and heat treatment parameters (cooling rate(CR) and tempering temperature(TT)). The outputs of the ANN model include property parameters namely: ultimate tensile strength(UTS), yield strength(YS), percentage elongation(EL), reduction in area(RA) and impact energy(IS). The model can be used to calculate the properties of low alloy steels as a function of alloy composition and heat treatment variables. The individual and the combined influence of inputs on properties of medium carbon steels is simulated using the model. The current study achieved a good performance of the ANN model, and the results are in agreement with experimental knowledge. Explanation of the calculated results from the metallurgical point of view is attempted. The developed model can be used as a guide for further alloy development. And also model can be used in web application that can be beneficial for Student or Company purpose.

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Chapter 1

Introduction

The design of alloy steels with the desired properties is a challenging task as it involves a multi-objective optimization of various problems. For example, it is hard to design a material that combines high strength and ductility, which are the two most key mechanical characteristics of metals. There are excellent facilities to measure the composition, microstructure, and properties. However, it is difficult to predict reliable mechanical properties with the comprehensive description of the chemical composition, processing parameters and structure of steels. The microstructure in steels determine the mechanical properties and the typical metallurgical approach for the prediction of properties through structure-properties relationships follows the hierarchy of composition and processing conditions – microstructure – mechanical properties

Developing models for the analysis of complex multicomponent steel properties is a difficult task as a quantitative treatment is necessary. Physical models are not capable of predicting the mechanical properties of steels. The first hurdle to overcome during modeling of steels is to acquire a reliable database. The industries that manufacture these alloys (or steels) tend to classify their process variables for obvious reasons. It is therefore very difficult to get a data set or information that would consist all of the above details. As the relationships between these outputs and inputs are nonlinear and complex in nature, it is impossible to develop them in the form of mathematical equations.

The conventional linear regression is not sufficient to describe the relationships; hence the biologically inspired artificial neural networks (ANNs) have been identified as appropriate tools. ANN models are well-known for function approximation and feature extraction of the highly complex non- linear relationships from the data. In the present approach, both the compositions and heat treatment variables which determine the microstructure

are related directly to the mechanical properties. Hence, it is appropriate to attempt these techniques to enable the quantitative expression and understanding of the complicated non-linear problem.

1.1 Objective

The objective of the present work is, to develop a neural network model, which can predict the mechanical properties for a given composition of metals and heat treatment, and the relationship of the properties with respect to these input variables.

1.2 ANN Model

ANN model is a combination of a mathematical function and associated weights between the inputs, hidden units and outputs. Experimental data are presented to the network in the form of input and output parameters, and optimized nonlinear relationship is found by minimizing mean square error. The error adjustment step takes place once the data is presented to the input layer and forward propagation is finished. Every processing element in the output layer estimates an output and compared with the actual output specified in the data set. An error value for every unit is calculated based on the difference. The weights of these units are adjusted based on the error for all of the interconnections established with the output layer. After this, the subsequent sets of weights are adjusted for the interconnections coming into the hidden layer located just beneath the output layer. Upon each presentation, the weights are adjusted to decrease the error between the network's output and the actual output. This process is continued until all the weights of the network are adjusted. ANN model captures complex interactions involving the input and output variables, which are difficult to visualize from an assessment of the weights. These optimized weights are stored in a matrix form in the model. The model is ready to make rapid predictions with the new data using the optimized weights, to plot the predictions, and to examine the metallurgical significance of the results. The back-propagation neural network is more commonly used for modelling many complex systems effectively. The application of ANNs in material science for evaluation of various phenomena has been reported earlier in many research reports.

Since, the ANNs are the computational models of learning and evolution process of natural intelligent system, the proposed framework is referred as computational intelligence. The computational intelligence models have been used to identify the quantitative relationships between the composition, heat treatment parameters and properties and to design the medium carbon steels for the desired mechanical properties.

Chapter 2

Requirements

2.1 Back-propagation neural networks (BPNN) modeling

A BPNN model consists of an input layer and an output layer with as many units as their respective number of variables. In-between the input and output layers are the hidden layers, each having a certain number of nodes (or units). The actual number of nodes depends heavily on the system and the acceptable error level of the model. The error-correction step takes place after a pattern is presented at the input layer and the forward propagation is completed. Each processing unit in the output layer produces a single real number as its output, which is compared with the targeted output specified in the training set. Based on this difference, an error value is calculated for each unit in the output layer. The weight of each of these units is adjusted for all of the interconnections that are established with the output layer. After this, the second sets of weights are adjusted for all the interconnections coming into the hidden layer that is just beneath the output layer. The process is continued until the weights of the first hidden layer are adjusted. As, the correction mechanism starts with the output units and propagates backward through each internal hidden layer to the input layer, the algorithm is called as back-error propagation or back propagation (BP). A BP network is trained using supervised learning mechanism. The network is presented with patterns, (inputs and targeted outputs), in the training phase. Upon each presentation, the weights are adjusted to decrease the error between the networks' output and the targeted output. A detailed description on BP algorithm used in the present study is beyond the scope of the present paper, and it can be found in literature. The training of the neural network has been carried out by using software developed in programming language C, and sigmoid function was used as an activation function with the BP training algorithm.

2.2 The steel under consideration

Typical applications of low alloy steels are general engineering components, high tensile bolts and studs, crankshafts, gears, boring bars, lead screws, shafting, milling and boring cutter bodies, collects. In the softened condition, the machinability of these steels is approximately 60% of that of mild steel, while in the hardened and tempered condition; the machinability is 45–55% of that of mild steel. The data on this low alloy steel has been collected from the handbook on Standard EN Steels. The data consists of the composition, i.e., the percentage of carbon, silicon, manganese, sulphur, phosphorous, nickel and chromium, as well as the section size, soaking temperature and type of quenching. The properties considered are the yield strength (YS), ultimate tensile strength (UTS), % elongation (EL), % reduction in area (RA) and impact strength (IS) in Joules.

The various heat treatment processes applied to low alloy steels are softening (subcritical annealing) at 650–690°C followed by air cooling or oil quench, hardening at 830–860°C followed by oil quench and tempering at 550–660°C followed by air cooling or oil quenching. The data consists of different section sizes and their heat treatment temperatures and type of quenching. So, the cooling rate varies for different section sizes, which is not uniform; furthermore, the variations of cooling rates are not linear. Based on ASM Metal handbook.

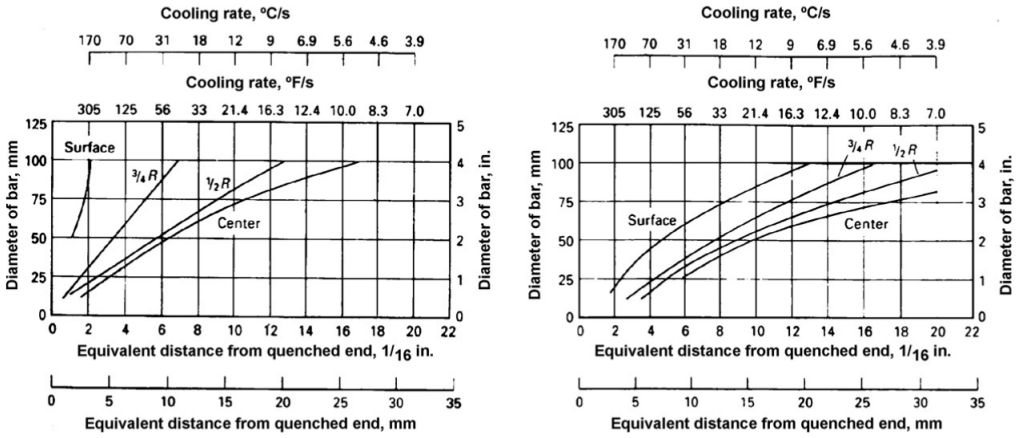

Figure 2.1: Cooling rates for (a) oil quenching and (b) water quenching from ASM Metals handbook.

The cooling rate equations were developed for different section sizes. The equations obtained based on the best fits are shown below.

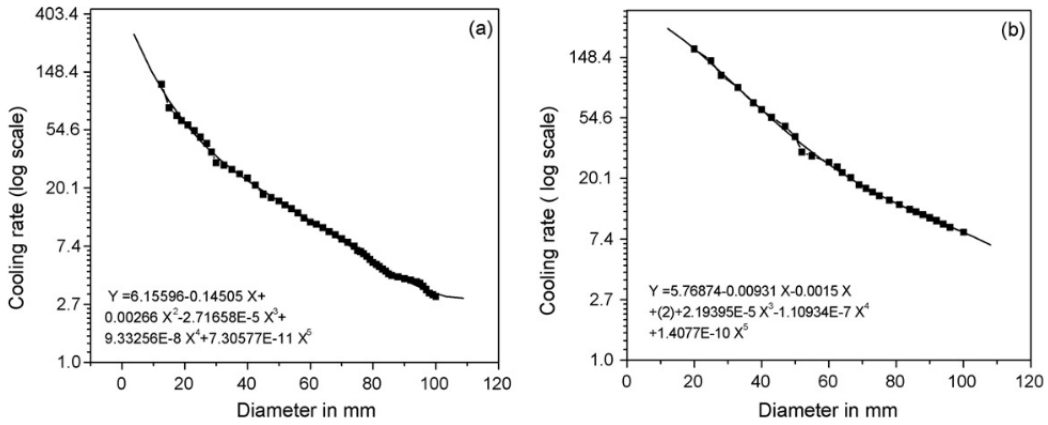

Figure 2.2: Cooling rates variation with diameter of the sample for (a) oil quenching and (b) water quenching.

For water quenching,

$$Y = 5.77 - 0.01X - 0.002\ X^2 + 2.19E - 5\ X^3 - 1.11E - 7\ X^4 + 1.41E - 10\ X^5$$

For oil quenching,

$$Y = 6.16 - 0.15X + 0.003\ X^2 - 2.72E - 5\ X^3 + 9.33E - 8\ X^4 + 7.31E - 11\ X^5$$

where, X and Y are diameter of the specimen and cooling rate, respectively.

Based on the above equations, the cooling rate has been calculated for different section sizes and used as one of input parameters for NN training. After coding, the total sets available for modeling are 140 and shown in Appendix. Among the 140 data sets available, 112 data sets have been used for NN training. When training a model, the choice of input variables is of great importance. Also, when a combination of these variables is believed to be of particular importance, the model can be improved by adding the combination as an explicit variable. The model was trained on the ratio of Mn and S, where the concentrations are in wt%. This is because sulphur reacts with manganese and forms MnS. To avoid biasing of the model, the individual variables making up the Mn/S ratio are also included, so that the direct influence of any of them can also be detected. The statistics of the steels data used for neural network modeling is presented in [Table 1].

Variables	Training data (112 data sets)				Testing data (28 data sets)			
	Minimum	Maximum	Mean	Standard deviation	Minimum	Maximum	Mean	Standard deviation
C	0.32	0.44	0.37	0.030	0.32	0.44	0.38	0.032
Si	0.19	0.37	0.27	0.044	0.19	0.36	0.26	0.053
Mn	0.33	1.51	0.91	0.520	0.33	1.51	1.27	0.340
S	0.01	0.042	0.033	0.010	0.01	0.042	0.03	0.010
P	0.02	0.038	0.031	0.005	0.02	0.038	0.031	0.006
Ni	0.56	1.08	0.82	0.131	0.56	1.08	0.82	0.127
Cr	0.21	0.57	0.44	0.073	0.21	0.56	0.42	0.109
Mo	0.11	0.25	0.17	0.030	0.12	0.25	0.18	0.034
Mn/s	7.86	150	37.27	34.32	7.86	145	52.6	33.90
Cooling rate	2.8	118	24.9	29.79	2.8	54	24.3	17.49
Tempering temperature	400	700	588.8	66.85	450	700	592.7	69.00
YS (MPa)	542.8	1193.6	798.3	147.7	547.4	1161.7	850.1	155.5
UTS (MPa)	707	1284.8	923.6	127.3	732.9	1295.5	972	125.00
EL (%)	13	28.5	21.4	3.430	14	29	20.25	3.310
RA (%)	32	67.5	56.9	6.190	31	64	54.3	7.210
Impact strength (J)	15	94	58.5	21.96	15	93	53.6	21.50

Table 2.1: Statistics of data used for neural network modeling.

Chapter 3

The Analysis

3.1 The training behavior of BPNN model

The results obtained from modeling studies are presented and discussed in detail. The optimal parameters of the network are determined based on the minimum mean sum square (MSE) error and the average error in output prediction (E_{tr}) of the trained data.

$$E_{tr}(x) = \frac{1}{N}\sum_{i=1}^{N}|T_i(x)\text{-}O_i(x)|$$

where $E_{tr}(x)$ = average error in prediction of training data set for output parameter x. N = number of data sets, $T_i(x)$ = targeted output, $O_i(x)$ = output calculated.

In applying the BPNN for the proposed estimation work, the following key design issues, i.e. number of hidden layers and hidden neurons, neural network parameters (learning rate and momentum rate) and number of iterations are discussed.

3.1.1 Choice of number of hidden layers and neurons in the hidden layer

The influence of the number of hidden layers and the number of neurons in each hidden layer on the convergence criterion is studied extensively. In order to decide the suitable number of hidden layers, two basic structures of the neural networks are examined: one

Neurons in layer 1	Neurons in layer 2	MSE	E_{tr} (YS)	E_{tr} (UTS)	E_{tr} (%EL)	E_{tr} (%RA)	E_{tr} (IS)
7	6	0.04178	45.50	32.12	1.08	3.93	7.73
7	8	0.05658	47.62	38.12	1.23	2.92	7.70
8	6	0.04140	51.19	39.26	1.17	2.35	6.95
8	7	0.02832	36.66	30.28	0.93	1.79	6.84
8	16	0.02613	39.05	29.91	0.95	2.03	5.84
8	32	0.00828	23.87	21.06	0.52	0.99	3.06
9	8	0.03171	41.38	30.72	0.84	2.40	6.14
10	20	0.01160	24.32	24.62	0.59	1.32	3.97
15	25	0.00723	28.70	24.38	0.41	0.54	2.36
16	18	0.00860	19.56	15.88	0.51	0.83	2.33
16	24	0.00585	23.73	20.48	0.53	0.57	2.46
16	32	0.00559	31.50	22.24	0.40	0.64	2.73
18	16	0.00848	23.89	22.17	0.56	0.71	2.35
20	10	0.01204	29.08	23.20	0.64	1.23	3.01
24	16	0.00685	22.81	20.95	0.41	0.64	2.17
25	15	0.00672	21.21	19.13	0.50	0.81	3.20
25	30	0.00568	23.29	18.09	0.31	0.37	1.73
30	25	0.00470	29.71	20.10	0.37	0.61	2.46
32	8	0.01215	28.00	25.37	0.72	1.20	2.70
8	8	0.02045	42.69	31.99	0.69	1.65	5.53
9	9	0.02313	38.07	28.60	0.83	1.50	6.10
10	10	0.02351	32.30	27.25	0.96	1.90	5.86
11	11	0.01517	28.19	22.44	0.84	1.32	4.27
12	12	0.01576	31.87	24.75	0.72	1.42	4.27
13	13	0.01272	24.75	22.62	0.59	1.21	3.46
14	14	0.01165	24.01	19.44	0.58	1.11	2.92
15	15	0.01039	25.51	22.39	0.55	0.90	3.45
16	16	0.00981	26.37	22.48	0.64	0.92	2.97
17	17	0.00880	26.67	21.87	0.50	0.73	2.59
18	18	0.00747	26.55	21.96	0.54	0.77	2.77
19	19	0.00672	21.19	16.96	0.47	0.67	2.46
20	20	0.00652	32.33	26.12	0.47	0.58	2.16
21	21	0.00677	23.40	17.68	0.36	0.50	2.18
22	22	0.00406	16.21	13.91	0.28	0.41	1.52
23	23	0.00596	19.53	17.34	0.34	0.60	1.97
25	25	0.00433	21.59	20.67	0.36	0.58	2.09
30	30	0.00359	22.45	21.57	0.36	0.59	2.21

Table 3.1: The variation of MSE as a function of hidden neurons. (η: 0.25, α: 0.9 and the number of iterations executed are 200,000).

with single hidden layer and the other with two hidden layers. In the first case, the BPNN structure of one hidden layer with a learning rate of 0.25 and a momentum rate of 0.9 was trained with different hidden neurons starting from 8 to 30. Eight hidden neurons in single layer yield a value of MSE of 0.02045 after 200,000 iterations. Fig:3.1 shows the variation of MSE and E_{tr} for different properties with the number of neurons in the hidden layer. With an increase in the number of neurons, the MSE value increases up to 10 hidden neurons and then gradually decreases with further increase of hidden neurons. In order to examine the effect of number of layers, the NN structure is also designed with two hidden layers, each containing 8–30 neurons in each layer, and the results are shown in Table 3.2. The effect of different combination of hidden neurons on two hidden layers is also shown in Table 3.1. Excellent convergence was observed with 22 hidden neurons in each layer, and a value of MSE of 0.00427 was obtained after 200,000 iterations with η: 0.25, α: 0.9.

From Fig: 3.1, it is clear that the convergence is better for the two hidden layers than the single hidden layer with different number of hidden neurons in the layer. Hence, 22

Number of iterations	MSE
500	0.09592
1,000	0.07067
5,000	0.01442
10,000	0.00943
20,000	0.00611
40,000	0.00464
50,000	0.00479
60,000	0.00461
75,000	0.00411
100,000	0.00237
125,000	0.00268
150,000	0.00149
175,000	0.00145
180,000	0.00104
185,000	0.00109
190,000	0.00107
195,000	0.00102
200,000	0.00102

Table 3.2: Variation of MSE of the trained data as a function of number of iterations (η = 0.55 and α = 0.65, number of hidden neurons = 22 and number of hidden layers = 2).

hidden neurons with two hidden layers have been selected for further training to optimise other parameters. Even though the MSE is 0.00359 with 30 hidden neurons, which is far less than that of 22 hidden neurons, the average error in output predictions is greater in all the mechanical properties. Hence, 22 hidden neurons in two layers were selected for analysis. One more advantage with the 22 hidden neurons selection is its less complexity in comparison to if 30 hidden neurons were to be selected.

3.1.2 Choice of neural networks parameters

For back-propagation learning algorithm with fixed values of learning rate, η, and momentum rate, α, the optimum values are obtained by simulation with different values of η and α. Two values, $\eta = 0.25$ and $\alpha = 0.9$, are initially chosen and varied to get the optimum value for each parameter. Fig: 3.2 shows the variation of MSE and E_{tr} for mechanical properties of the training data for different values of η and α with two hidden layers consisting of 22 hidden neurons in each layer. From Fig: 3.2, it is clearly evident that larger value of learning rate results in higher MSE and E_{tr}, which is an expected behavior. This phenomenon is usually referred to as over training. However, it was observed that with

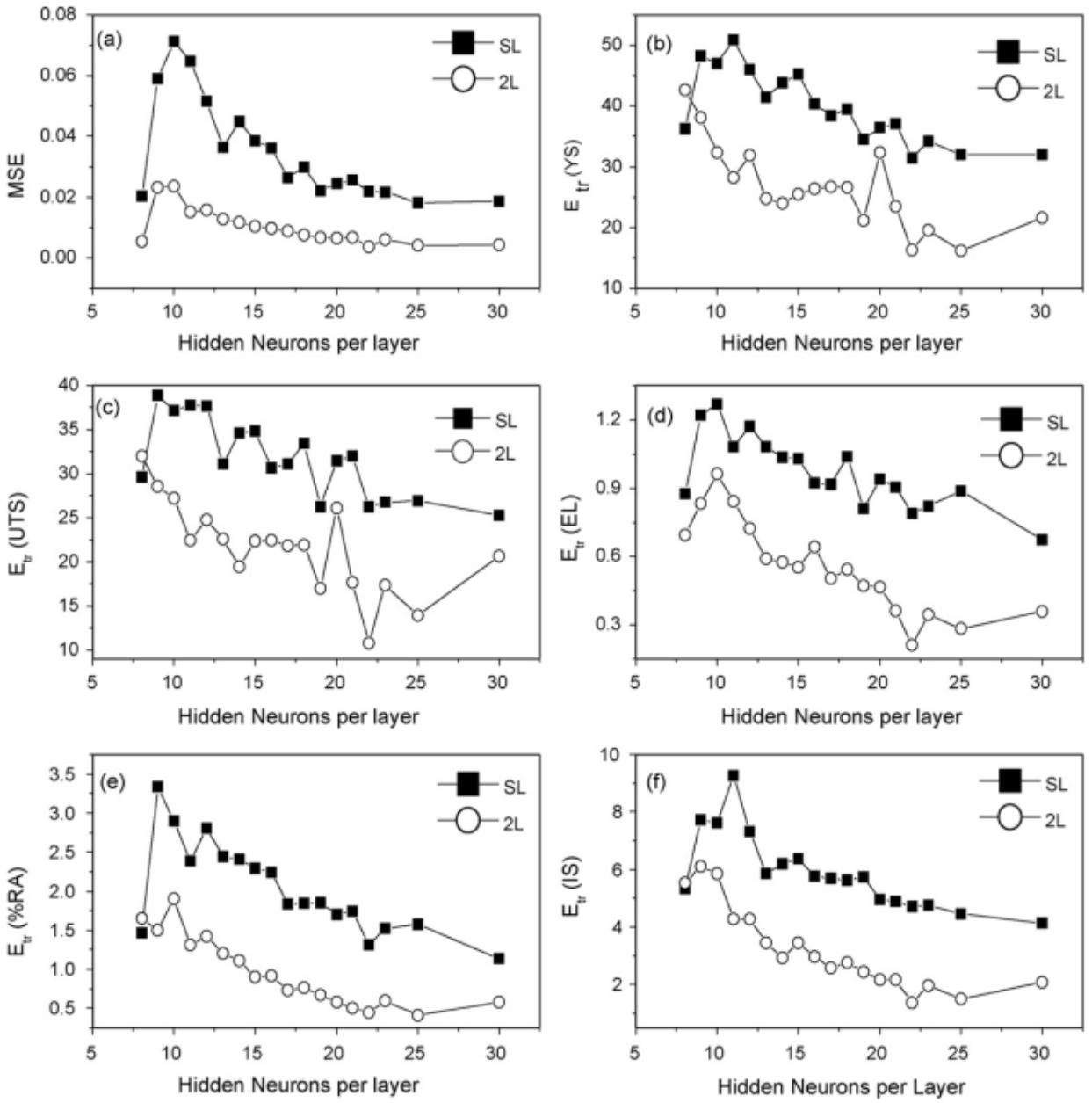

Figure 3.1: Variation of (a) MSE and average error in output prediction (E_{tr}) of (b) YS, (c) UTS, (d) EL, (e) RA and (f) IS of the train data as a function of the number of hidden neurons with single hidden layer and two hidden layers.

higher learning rates, the convergence takes place faster than it does at lower learning rates. The figure also indicates that MSE and E_{tr} are not quite sensitive to the momentum rate. The best combination is found to be when η is 0.55 and α is 0.65 (Fig: 3.2). For the above combination, the MSE of 0.001015 is obtained after 200,000 iterations.

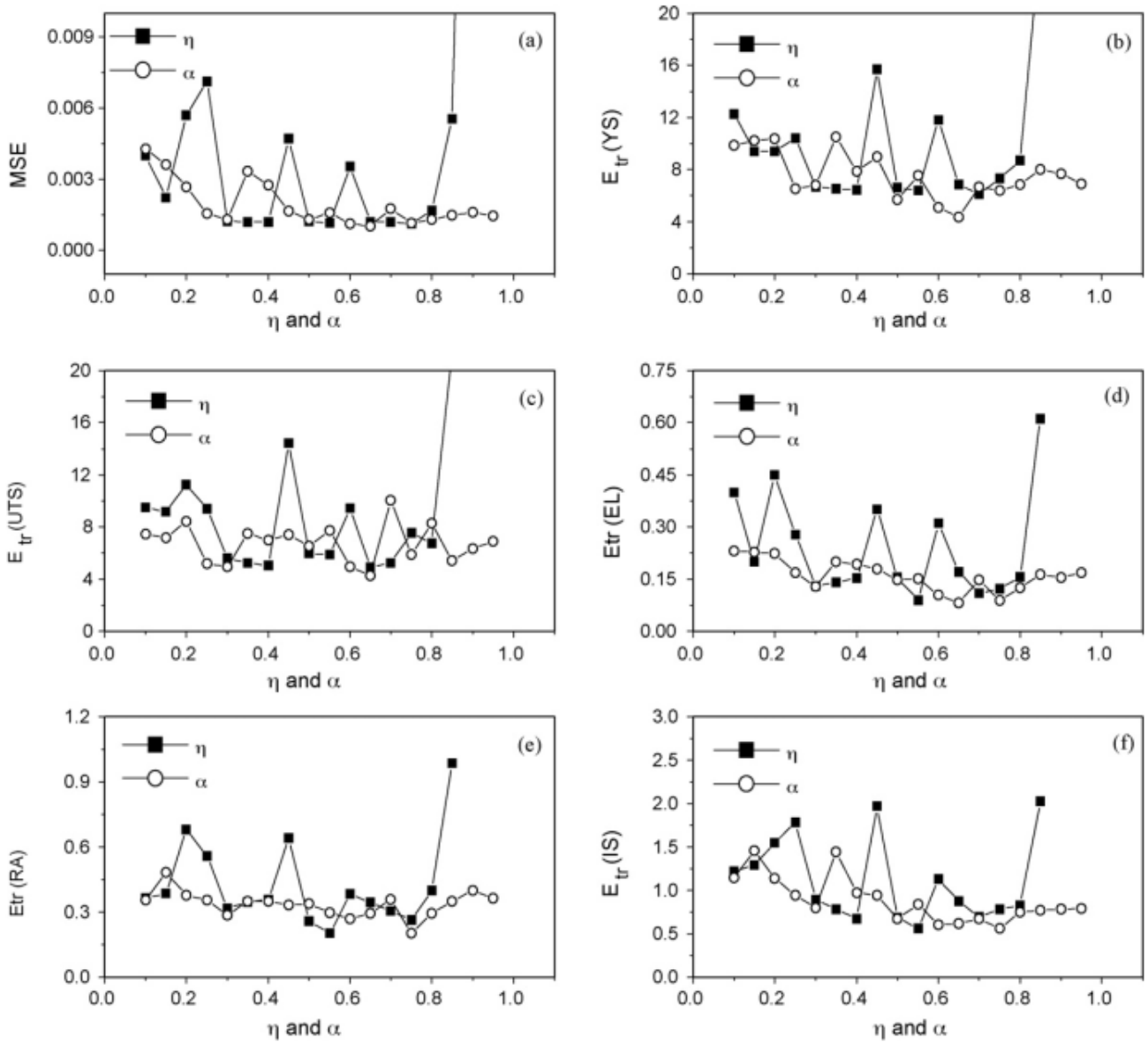

Figure 3.2: Variation of (a) MSE and average error in output prediction (E tr) of (b) YS, (c) UTS, (d) EL, (e) RA and (f) IS of the train data as a function of learning rate and momentum rate in the steps of 0.05.

3.1.3 Number of iterations

The number of iterations executed to obtain optimum values is an important parameter in the case of BPNN training. The MSE achieved from different iterations is shown in

Table 3.1. It is evident that the value of MSE gradually decreases during the progress of training, as expected. An error of 0.07067 after 1000 iterations reduces to 0.00237 after 100,000 iterations and falls to 0.00104 after 180,000 iterations, and no change has been found with further increase in the number of iterations. It has been observed that the MSE does not change significantly beyond 200,000 iterations and hence further processing has been stopped after the abovementioned iterations. Finally, the 11 units in input layer, 22 hidden neurons in two hidden layers and 5 units in output layer (11-22-22- 5) architecture with a learning rate of 0.55 and a momentum rate of 0.65 are used for prediction and analysis of the EN100 steels.

3.2 Predictions of test data sets

Total data sets available for BPNN Model training is 140. The randomly selected 112 data sets have been used for training, and the remaining 28 data sets are used for testing.

The predictions of 114, 115, 116, 118, 119, 123, 125, 127, 128, 131, 133, 136, 137, 138 and 140 data sets (a total of 15 sets) are presented in Fig: 3.3(a), (c), and (e). The comparison between the actual and predicted values and the respective percentage error for 15 testing data sets is also shown in Fig: 3.3(b), (d), and (f). It has been observed that most (nearly 95%) of the outputs predicted by the model are within 4% of the error band (indicated in Fig:3.3 6(b), (d) and (f)). For the testing data that has never been seen by the model, the NN gives a reasonably accurate prediction. In the case of sample 11 (data set of 133), it can be seen that there is a less variation between actual and predicted values as shown in Fig:3.3(e), but the percentage error is higher because the actual values are very small.

3.3 Hypothetical alloys

The developed model can be used in practice to manipulate the mechanical properties of EN100 steels, in general, by altering chemical composition and heat treatment variables. The effects of all of these can be estimated quantitatively by using the BPNN model to observe whether they make any metallurgical sense. The combined effect of a single variable or any two variables on the properties has also been studied. Here we present some hypothetical alloys by varying the composition and heat treatment variables and their effect on mechanical properties namely: (a) yield strength (YS), (b) ultimate tensile strength (UTS), (c) % elongation (EL), (d) % reduction in area (RA) and (e) impact strength (IS) for sample

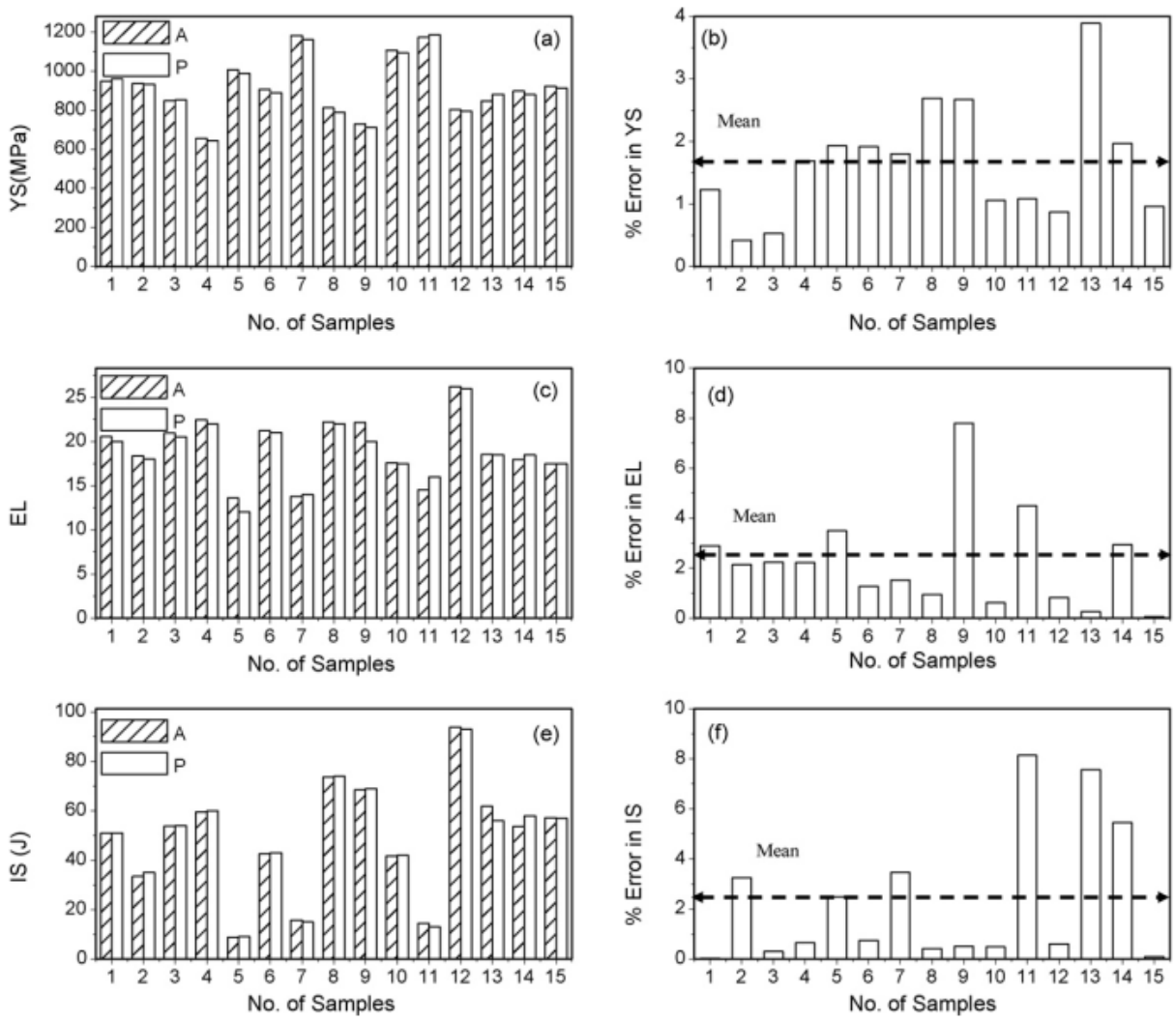

Figure 3.3: The comparison of actual (A) and predicted (P) values and the respective percentage errors for 15 test samples of EN100 steels. (a) and (b) YS, (c) and (d) EL and (e) and (f) IS.

number 91 of Appendix is presented in Figs.3.4-3.6. The effect of combined variation of two elements on properties is presented in Figs.3.7 and 3.8. The composition of sample 91 is given in Table 3.3.

3.3.1 Effect of carbon on properties

Carbon is an essential non-metallic element in iron to make steel. None of the other elements so dramatically alters the strength and the hardness as do small changes in the carbon content does. Carbon is the principal hardening element, influencing the level of hardness

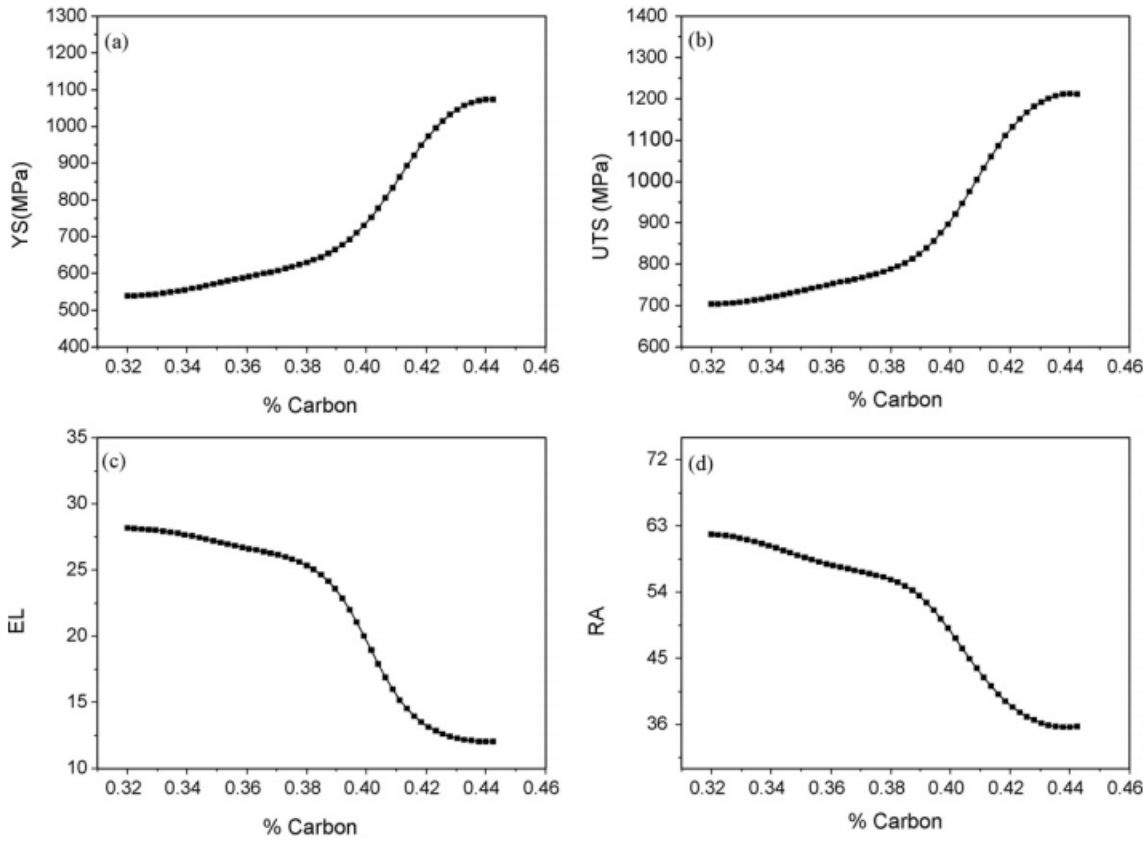

Figure 3.4: Effect of carbon variation on mechanical properties of sample 91: (a) YS, (b) UTS, (c) EL and (d) RA.

S. no.	S91
C	0.4
Si	0.3
Mn	1.51
P	0.034
Ni	0.89
Cr	0.21
Mo	0.16
Mn/S	41.94
CR	3.1
Temp.	550

Table 3.3: Composition and heat treatment variables of sample 91.

or the strength attainable by quenching. The model predictions as indicated in Fig.3.4 show that the YS and UTS increase while the EL and RA decrease with increase in C content.

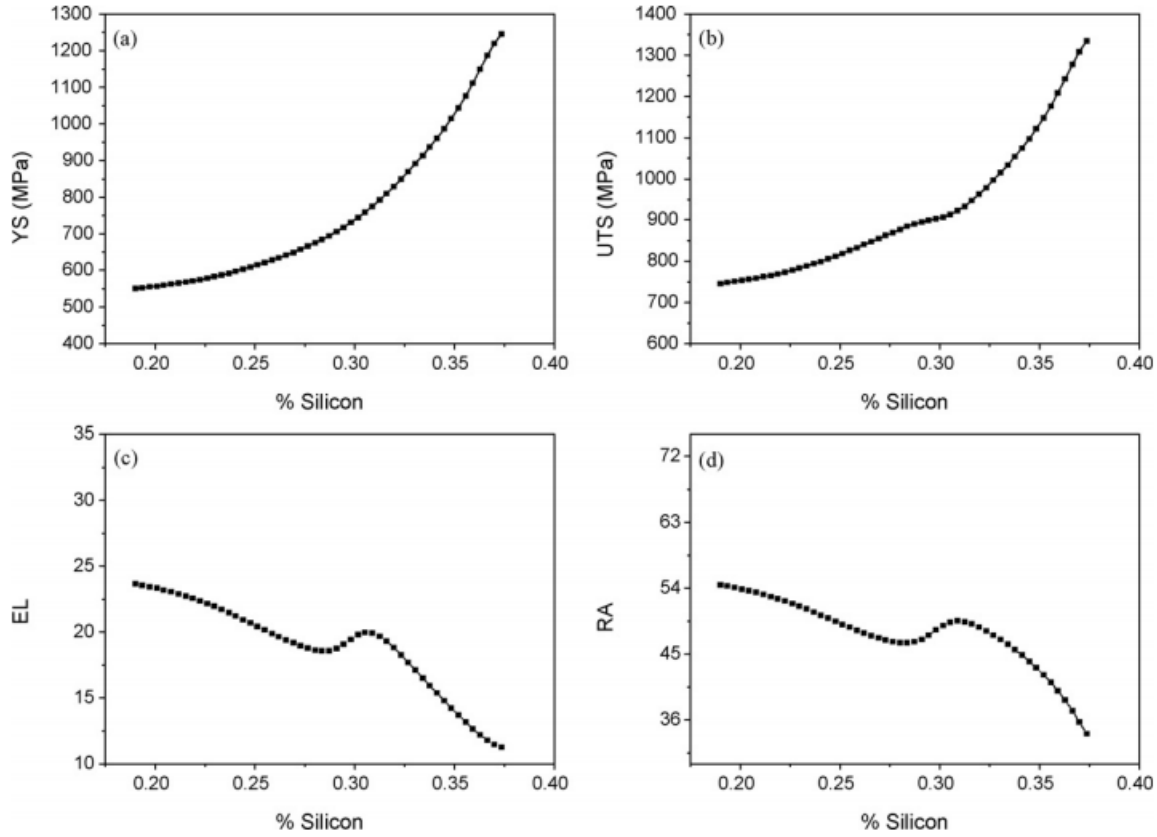

Figure 3.5: Effect of silicon variation on mechanical properties of sample 91: (a) YS, (b) UTS, (c) EL and (d) RA

As carbon increases from 0.32% to 0.44%, (Fig.3.4), there will be approximately a 15% increase in the formation of pearlite accompanied by a reduction of ferrite by the same amount, which results in an increase in strength and a decrease in ductility. The increase in strength and the decrease in ductility with the increase in carbon content are also due to the increase in the formation of various carbides with the other alloying elements as the carbon percentage is increased from 0.3 to 0.44. The impact strength would also decrease, as the area under the stress–strain curve would decrease owing to the reduction in ductility. Thus, the predictions of Fig.3.4 are clearly is in agreement with the expected experimental trend.

3.3.2 Effect of silicon on properties

Silicon is one of the principal deoxidizers used in steel making and therefore the amount of silicon present is related to the type of steel. Usually only small amounts (0.20%) are

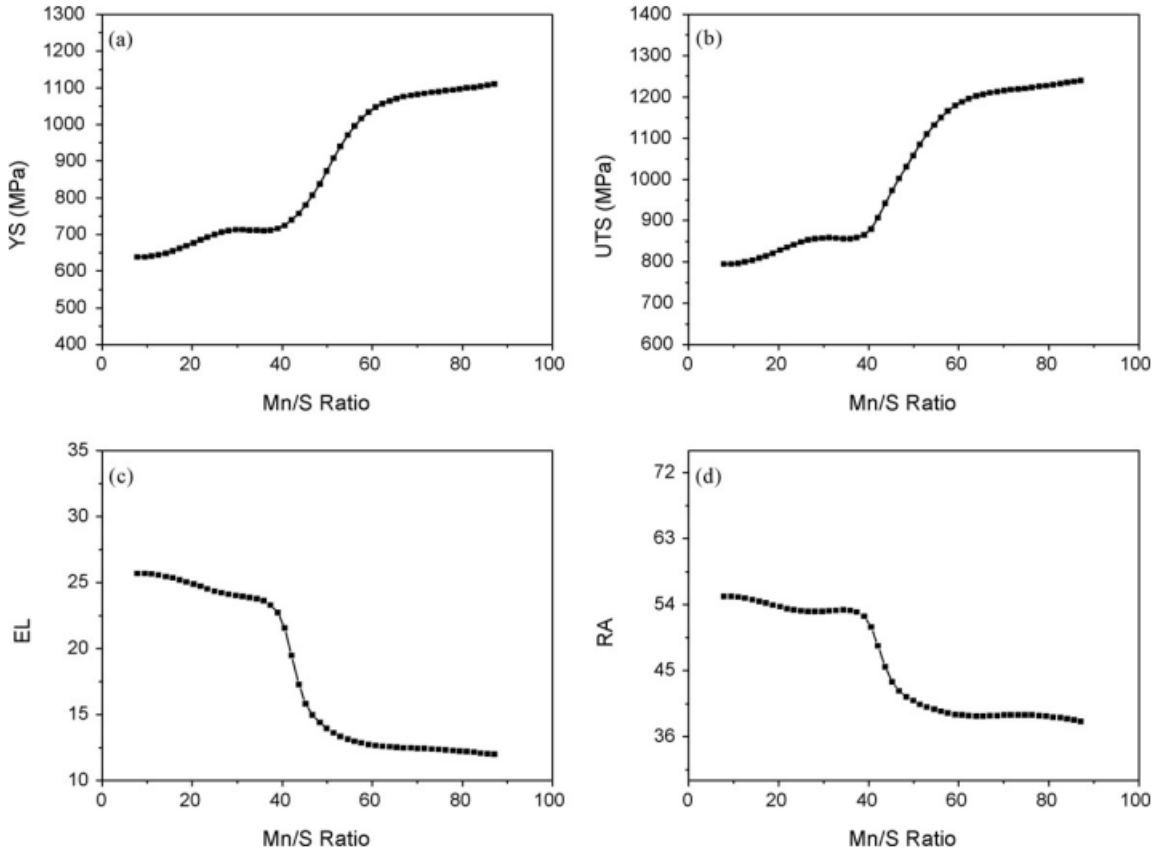

Figure 3.6: Effect of Mn/S variation on mechanical properties of sample 5: (a) YS, (b) UTS, (c) EL and (d) RA.

present in rolled steel when it is used as a deoxidizer. Silicon dissolves in iron and tends to strengthen it. In the low alloy steels, Si is present in the range of 0.2–0.4%. Fig. 8 shows the variation of mechanical properties with silicon content in the range of 0.2–0.4%. The variation in mechanical properties as observed in Fig.3.5 cannot be explained based on the effect of Si alone. It is possible that a number of other elements present might be responsible for the behavior represented in Fig.3.5. Fig.3.5 shows that a significant change occurs in mechanical properties at around 0.3% Si, which needs to be explained based on metallurgical principles involving the complex combined effects of a number of elements. However, it is important to note that a significant increase in the UTS at around 0.3% Si brings a significant reduction in EL and RA exactly at the same composition. This suggests that the model is able to establish strong correlations between the individual output parameters, though such information is not fed to the model a prior.

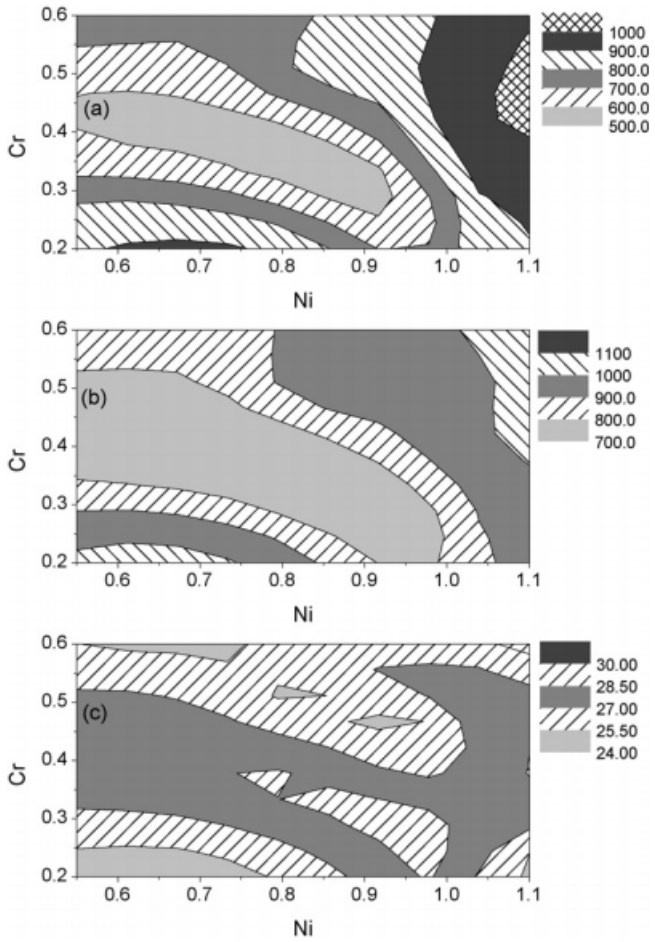

Figure 3.7: Combined effect of Ni and Cr variation on mechanical properties for sample 91: (a) YS, (b) UTS and (c) EL

3.3.3 Effect of Mn/S ratio on properties

Manganese is a deoxidizer and degasifier, which reacts favorably with sulphur to improve forging ability and surface quality as it converts sulphur to manganese sulphide. Manganese increases tensile strength, hardness, hardenability, and resistance to wear and increases the rate of carbon penetration during carburizing. There is a tendency nowadays to increase the manganese content and reduce the carbon content in order to achieve steels with an equal tensile strength but improved ductility. Fig.3.6 shows the effect of Mn/S variation on mechanical properties. As Mn/S ratio increases strength increases with a corresponding reduction in ductility, which is clearly brought out by the model in Fig.3.6

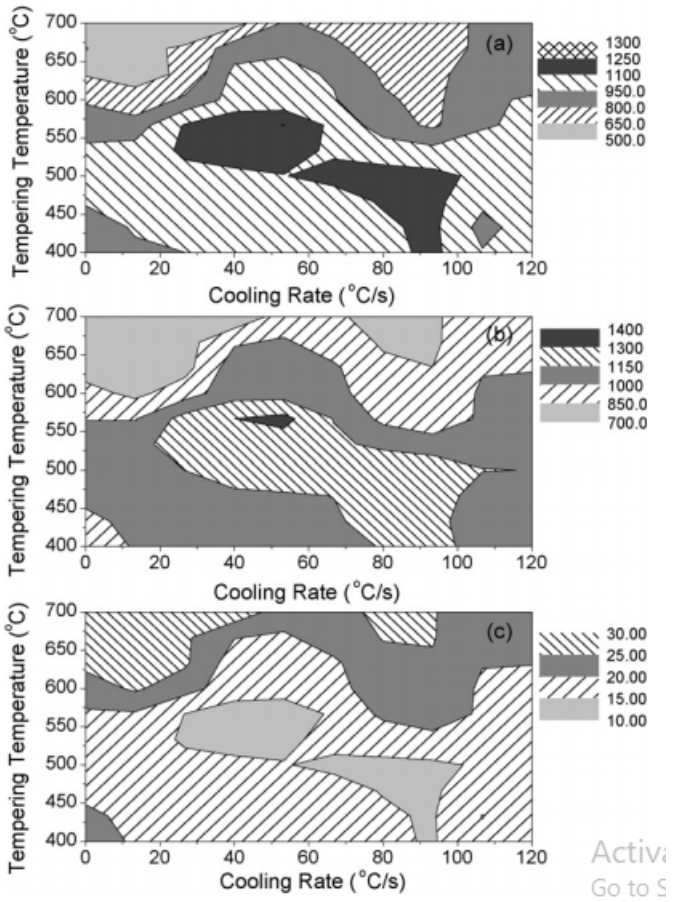

Figure 3.8: Combined effect of cooling rate and tempering temperature variation on properties for sample 91: (a) YS, (b) UTS and (c) EL.

3.3.4 Effect of nickel and chromium on properties

Nickel is used to stabilise alloy steels. Nickel and manganese exhibit very similar behavior and both lowers the eutectoid temperature. It strengthens ferrite by solid solution but is a powerful graphitiser. Nickel increases the impact strength of engineering steels considerably. It increases the strength and hardness without sacrificing ductility and toughness. Steels with 0.5% nickel is similar to carbon steel but is stronger because of the formation of finer pearlite and the presence of nickel in solution in the ferrite. Among all of the common alloying elements, chromium ranks near the top in promoting hardenability. It makes the steel apt for oil or air hardening as it reduces the critical cooling rate required for the formation of martensite. Fig.3.7(a)–(c) shows combined effect of Cr and Ni on the YS, UTS and EL, respectively. The figure clearly points out that the YS and UTS decrease with an increase in Cr content at lower concentrations for a given Ni concentration, which can be attributed to the ferrite stabilisation. However, at higher Cr content, the strength starts to

increase again due to the formation of carbides. The percentage elongation shows exactly the opposite trend, as expected. Thus, the model is able to predict the combined effect of Ni and Cr quite successfully.

3.3.5 Combined effect of cooling rate and tempering temperature on properties

The effect of cooling rate on properties is non-linear and complex, and it is difficult to explain. Fig.3.8(a)–(c) shows the combined effect of cooling rate and tempering temperature on the YS, UTS and EL, respectively. Increase in tempering temperature brings in an initial increase in the strength in the temperature range of 450–550°C, which could be attributed to the secondary hardening. Further increase in the tempering temperature leads to a decrease in the strength, as expected. The EL shows a reverse trend as expected. It is also important to note that the variation in the mechanical properties is larger with different heat treatment parameters (cooling rate and tempering temperature), in comparison to that with Cr and Ni variation. This clearly suggests that the mechanical properties are more sensitive to heat treatment parameters than the concentration of alloying elements such as Cr and Ni, which is clearly predicted by the model. Table 5 shows actual and model predicted mechanical properties for different hypothetical alloys for sample 91. Though it is difficult to explain each and every behavior of hypothetical predictions, the model predicted a sudden increase in ductility, whenever there is a sudden decrease in the strength and vice versa, which has to be noted. It is very much clear that the error in the model predictions is less than 4% in all cases. This shows the efficiency of the model in understanding the relationships between input parameters and output parameters. This will greatly help the designing of alloy to achieve certain target properties.

Hypothetical alloy	Fig. no.	Mechanical properties (experimen	
		YS	UTS
Sample 91 (experimental)		760	931
Carbon (0.4)	7	753	921
Silicon (0.3)	8	737	906
Manganese (1.51)		738	905
Phosphorous (0.034)		736	901
Nickel (0.89)		738	906
Chromium (0.21)		737	904
Molybdenum (0.16)		734	904
Mn/S ratio (41.94)	9	739	907
Cooling rate (3.1 °C/s)		724	916
Tempering temperature (550 °C)		737	904

Table 3.4: Comparison of actual and predicted properties for hypothetical alloy of sample 91.

Chapter 4

Conclusions

4.1 Conclusion

1. A comparison of the modeled and experimental results indicated that NN can very well be employed for the estimation and analysis of mechanical properties as a function of chemical composition and/or heat treatment for low alloy steels.

2. Two hidden layers converged better than the single hidden layer.At higher learning rate, the MSE and Etr significantly increased as expected.

3. Even though Rumelhurt et al.Suggested that a learning rate, $\eta = 0.25$,and a momentum rate, $\alpha = 0.9$, yield good results for most applications, the present work indicated it is not always so, and that the optimum values vary for different steels. This fact was in agreement with the finding of Satish and Zaengl and Chakravorti and Mukherjee. The best combination of ANN parameters for the best results in each case studied was identified.

4. Present model was able to map the relation between the output parameters, even though such a relation was not explicitly fed to the model. For example,the relationship between ductility and strengths was clearly brought out by the model.

5. Results from the current study demonstrated that the neural network model can be used to examine the effects of individual input variables on the output parameters, which is incredibly difficult to do experimentally.