The Iraqi Journal For Mechanical And Material Engineering, Vol.11, No.4, 2011

PREDICTION OF YIELD STRENGTH OF LOW/MEDIUM CR-MO FERRITIC STEELS USING ARTIFICIAL NEURAL NETWORKS

R. M. Hussein*, N. J. Hammadi** and Q. A. Rishaq**

Abstract

The yield strength of Low/Medium Cr- Mo ferritic steels has been analyzed by a well selected artificial neural networks (ANN) model using data sets obtained from ASTM publications. The qualitative and quantitative effects of chemical composition, heat treatment and test temperature have been studied. The proposed ANN model was obtained by applying averaging process to the first best three models. The first one consists of 24 input nodes (the input variables), 23 hidden nodes and the output node which is the target for the required yield strength. Among the previous variables, it was found that the heat treatment ones have the greatest contribution to the yield strength especially the tempering one i.e. the average contribution of about 15% was obtained.

Keywords: yield strength, ferritic steels, artificial neural networks, 2¼Cr-1Mo steels, averaging process.

الخلاصة

تم تحليل مقاومة الخضوع للصلب الفرايتي الواطئ والمتوسط Cr–Mo من خلال اقتراح موديل مناسب من الشبكات العصبية الصناعية. تم دراسة التأثيرات النوعية و الكمية للتركيب الكيميائي و المعاملة الحرارية و درجة حرارة الاختبار على مقاومة الخضوع باستخدام مجموعة بيانات مأخوذة من نشرات ASTM. تم الحصول على النموذج المقترح بتطبيق طريقة المعدل لأفضل ثلاث موديلات. إن أفضل موديل من بين هذه الثلاثة كان يتكون من 24 عقدة في الطبقة الأولى (المتغيرات) و 23 عقدة في الطبقة المخفية وعقدة واحدة للهدف المطلوب و هو مقاومة الخضوع في الطبقة الأخيرة. لوحظ بان متغيرات المعاملة الحرارية ذات تأثير اكبر على مقاومة الخضوع مقارنة مع المتغيرات الأخرى و بالأخص متغير درجة حرارة معاملة التطبيع حيث تم الحصول على معدل تأثير بمقدار 15%.

* Dep. of Mech. Engg. , University of Basrah.

** Dep. of Mat. Engg. , University of Basrah.

Introduction

In high temperature environments not lower than 400°C austenitic stainless steels, high Cr steels with a Cr content of 9 to 12 %, low/medium Cr steels and carbon steels have been used selectively in respective matched fields. Among the various steels mentioned above, low/medium Cr steels contain more amounts of Cr than carbon steels and therefore they are superior in oxidation resistance, high temperature corrosion resistance, strength at elevated temperatures and creep strength.Furthermore, although low/medium Cr steels are inferior to austenitic stainless steels in strength at elevated temperatures or creep strength, they have smaller thermal expansion coefficient, much more inexpensive and characterized by superior toughness, weldability and thermal conductivity [Kawano, K., 2003].

There have been numerous attempts to model metal mechanical properties using linear regression analysis. The developed linear equation may contain non-linear terms, forming a pseudo-linear equation. **The strength of a metal is frequently modeled as functions of chemical composition in which** the form of the equation has to be specified before performing the analysis **[**Lalam, S., H., 2000**].The following model is an example in which alloying elements are based on weight percent:**

$$YS = 104.1 + 32.6\ Mn + 84\ Si + 17.5\ d^{-1/2} \quad (1)$$

Where YS and *d* represent yield strength in MPa and grain size in μm for steels having an essentially ferritic microstructure [Vodopivec, F., 2007]. It should be mentioned that the stress-strain curves of ferritic alloys don't show a well defined yield point, so the term yield strength refers to 0.2% offset yield strength.

Artificial neural networks (ANN)are computational networks that attempt to simulate those processes occurring in the human brain and nervous system that enable pattern recognition, information filtering and functional control. They are part of a larger group of methods used for data mining *i.e.* the use of databases to extract models to classify or predict classes or trends. Decision trees, Bayesian belief networks, regression analysis, fuzzy logic and neural networks are all examples of data mining methods [Dunne, D.; 2004].

Modeling mechanical properties of ferritic steels by ANN has been studied by many researchers. Cole and Bhadeshia 1999 [Cole, D., 1999] and Murugananth 2002 [Murugananth, M., 2002] investigated the modeling of creep rupture strength of ferritic power plant steels as a function of chemical composition, heat treatment, test temperature and time. Also, Murugananth 2002 [Murugananth, M., 2002] studied Charpy toughness, elongation and ultimate tensile strength and yield strength of ferritic steel welds. Dimitriu and Bhadeshia 2007 [Dimitriu, R. C., Apr.2007 and Dimitriu, R. C., Sep.2007] developed a single hidden layer ANNs model to predict the hot strength of ferritic steels as a function of chemical composition and heat treatment variables.

The purpose of the present work is to exploit the modeling capabilities of neural networks in the prediction of yield strength of ferritic steels based on composition, heat treatment and test temperature variables using the data of experimental work carried out by ASTM (refer to Table 1).

Neural Networks Modeling

The essentials of using ANNs in the modeling field have been studied in many researches and text books such as [MacKay, D., 2003, Baughman, D.R. 1995 and Simpson, P., 1990]. In general, there are two methods of learning neural networks: supervised and unsupervised learning. Supervised networks are the networks in which data is given in the form of inputs and targets, unsupervised networks are given data in the form of inputs only , then the network could be used to discover patterns in the inputs to transfer the high dimensional inputs into low dimensional ones [MacKay, D., 2003]. In supervised networks after selecting the training data and testing data, the program sets automatically the initial values of the weights (the model parameters) and calculates the predicted values of strength for both data sets. Then the training and testing errors (RMS error) are calculated between the predicted strength and the true strength (strength in data). The aim of the program is to reduce the testing error to minimum value which means obtaining the required model (refer to Fig.7-a). It should be mentioned that the neural model includes a huge number of weights (parameters) so it isn't suitable to put on papers and use it manually so it needs a computerization. Also the program (algorithm) needs to define two values concerning the training process: momentum coefficient and learning rate (both take the range of values between 0.0 and 1.0 and need to be tried to find the suitable value).

In the present analysis, supervised method has been used after preparation of the data concerning the ferritic steels shown in Table 1.

Selection of the Best Model

In this work the software package of Qnet 2000 (version 2K) for WINDOWS [Vesta Services, Inc., 2000] is used to conduct the ANNs models. After changing the necessary variables (momentum and learning rate) and using the same size of data for training and testing (50% of the total data for each), a number of 60 models has been generated. The best model configuration among the whole models was 23 hidden nodes with sigmoidal transfer function. The process of averaging is used to get the committee models over the first best ten models as cited in ref. [Bhadeshia, H., K., D., H., 1997]. This process is done after creating the suitable program using FORTRAN 90 language (refer to Fig.7-b). The first best three models when have been averaged, give the final model as shown in Fig.1.

Results and Discussion

The best model predictions when checked (using Qnet 2000 software) against the contributions of each input node (shown in Table 1), have resulted in the histogram shown in Figure 2. The differences between the effect of heat treatment variables and the others are noticeable. These differences tend to tell us that the input nodes of heat treatments are more effective in the value of yield strength of ferritic steels than the other nodes. Regarding the categorized nodes (16, 18, 20 and 22 in Table 1), one can conclude that they are not highly correlated with the other heat treatment ones i.e. their contributions are not small as compared to the related heat treatment temperature node. For the present steels the histogram shows that tempering temperature is the most affecting node. As we know in practice that increasing tempering temperature or time decreases the strength because of the variations in the type of carbide and or its concentration (refer to Fig.2).

Metallurgical Aspects

As mentioned previously, the heat treatment nodes have significant effect on strength rather than the alloying elements nodes and the tempering temperature node has the greatest effect among the other heat treatment ones.

To explain the relative importance of each node from the metallurgical point of view, the following rules will be presented.

Most of the alloying elements (nodes) such as: C, Mn, Si, Ni and Cu don't show a significant effect on yield strength in the short term of use or test of the steel (tensile test is a short term test). Its effects on the strength are remarkable in the long term of testing or using (creep phenomenon) [Komai, N. 2002 and Fujimitsu, M., 1991]. Mo and Cr in the long term may lead to the coarsening of carbides they form thus facilitate the movement of dislocations i.e. reduces the strength [Komai, N. 2002].

Some elements (nodes) such as Sn, Zr and Al are added to steel to get certain properties such as deoxidization or suppression of impurities effects (P and S) rather than the gain of strength [Miyata, K. 1997 and Nobuyoshi, K., 1998].

In view of the foregoing, the results of the present model concerning the alloying elements are matched to a great extent.

To explain the effects of heat treatment temperature nodes, if a certain steel of specified chemical elements (nodes) is taken. Austenising temperature of quenching or normalizing or full annealing is a certain temperature depends on the steel composition only [Gorni, A., A., 2007]. The range of changing this temperature is so small for a given steel and nevertheless it wouldn't change the resulted structure to a great extent. Thus, the existence of this node has its effects but the change of it wouldn't affect the strength remarkably.

Annealing temperature node in the range less than that of austenising (less than the range of full annealing) is so dependant on the previous state of the steel such as casting, welding and cold working and so on [Higgins, R., A., 1999]. Thus, it depends on variables out of the variables of the present model so its effect would be rather small as compared to the other heat treatment ones.

Finally, the node regarding tempering temperature existence and change has a wide range of effects because of the significant effects on the resulted microstructure (refer to Fig. 2). The mechanical properties are known to be susceptible to the microstructural changes, so these properties are so dependant on the tempering temperature node.

Table 1- Input parameters and their ranges for the present ANNs [Sturrock, C.P., 1995 and Armanios, E.A., 1997].

№	Input Variables	Minimum	Maximum
1	%C	0.05	0.27
2	%Si	0.0	1.55
3	%Mn	0.17	0.81
4	%P	0.0	0.03
5	%S	0.0	0.29
6	%Ni	0.0	0.62
7	%Cr	0.69	9.54
8	%Mo	0.0	1.3
9	%Cu	0.0	1.3
10	%Al	0.0	0.8
11	%N	0.0	0.025
12	%V	0.0	0.026
13	%Sn	0.0	0.04
14	%Zr	0.0	0.077
15	%Ti	0.0	0.54
16	Annealing (An) [a]	0 (off)	1(on)
17	Annealing Temperature (°C) [b]	690.56	1148.89
18	Normalizing (Nr) [a]	0 (off)	1(on)
19	Normalizing Temperature (°C) [b]	843.3	1148.89
20	Tempering (Te) [a]	0 (off)	1(on)
21	Tempering Temperature (°C) [b]	565.56	815.56
22	Quenching (Q) [a]	0 (off)	1(on)
23	Quenching Temperature (°C) [b]	621.11	1065.56
24	Test Temperature (°C)	21.11	982.22

[a] The variable here refers to a switch (off or on).

[b] The range of this variable concerns value of 1 (on) for previous binary variable.

Comparative Case Study

The present ANN model predictions have been compared with that of Dimitriu neural model [Dimitriu, R. C., Sep., 2007] as based on the experimental work cited in ref. [Sangdahl, G. S., 1982].

These experiments (Tables 2 and 3) have not been used in the present model training or testing. The input variables and their ranges of Dimitriu model are shown in Table 4.The results of comparison are shown in Figures 4, 5 and 6.

Conclusions

In the present case, the use of ANN has been successfully managed in the prediction of the yield strength of ferritic steels as a function of chemical composition and heat treatment parameters. For a given ferritic alloy in the range of this study, heat treatment variables especially the tempering one play a dramatic role in the final strength with a contribution of 15% which is much greater than that of the other variables. The comparison with Dimitriu model showed good superiority of the present one and near the lower bound of error for the selected 2¼Cr-1Mo steels plates.

Table 2- Chemical analysis of the plates 2, 4 and 7 as cited in ref. [Sangdahl, G. S., 1982].

	Chemical Analysis									
Plate №	%C	%Si	%Mn	%P	%S	%Cr	%Mo	%Ni	%Al	%Cu	%Sn
2[(a)]	0.13	0.23	0.52	0.011	0.021	2.23	0.95	0.18	0.031	0.17	0.012
4[(a)]	0.13	0.21	0.48	0.011	0.023	2.13	1.0	0.08	0.003	0.1	0.006
7[(a)]	0.1	0.21	0.48	0.012	0.023	2.39	0.95	0.23	0.003	0.18	0.012

[(a)] normalized at 900°C for 12 hour and tempered at 690°C for 12 hour.

Table 3- Tensile test results of the plates 2, 4 and 7 as cited in ref. [Sangdahl, G. S., 1982].

Plate №	Test T(°C)	21	316	371	427	482	538	593
2	TS(MPa)	528	425	433	424	404	342	261
4		524	447	457	446	413	370	286
7		509	379	392	398	380	333	253
2	YS (MPa)	298	246	258	252	243	219	198
4		296	264	265	291	254	257	220
7		283	233	212	210	220	207	185
2	%EL	24	21	19	21	21	26	36
4		26	20	19	21	21	24	33
7		27	25	21	21	23	24	37
2	%RA	40.4	59.9	55.8	57.6	60.2	67.5	82.0

4		60.0	59.0	58.9	64.3	66.3	73.6	82.6
7		67.1	63.5	60.0	60.6	62.6	69.4	82.7

Table 4- Variables used for predicting YS of Dimitriu model [Dimitriu, R. C., Sep., 2007].

№	Variable	Minimum	Maximum
1	%C	0.09	0.34
2	%Si	0.18	0.86
3	%Mn	0.38	1.44
4	%P	0.01	0.03
5	%S	0	0.02
6	%Ni	0	0.6
7	%Cr	0	12.38
8	%Mo	0.01	1.05
9	%Cu	0	0.25
10	%Al	0	0.04
11	%N	0	0.04
12	%V	~	~
13	%Sn	~	~
14	%Zr	~	~
15	%Ti	~	~
16	Annealing (An) [(a)]	~	~
17	Annealing Temperature (°C) [(b)]	~	~
18	Normalizing (Nr) [(a)]	~	~
19	Normalizing Temperature (°C)	~	~
20	Tempering (Te) [(a)]	~	~
21	Quenching (Q) [(a)]	~	~
22	Quenching Temperature (°C) [(b)]	~	~
23	Austenising time (min.)	10	540
24	Tempering time (min.)	30	660
25	Austenising temperature (°C)	870.15	970.15
26	Tempering temperature (°C)	625.15	750.15
27	Test temperature (°C)	20.15	700.15

[(a)] **The variable here refers to a switch (off or on).**

[(b)] **The range of this variable concerns value of 1 (on) for previous binary variable.**

~ : not specified in this model.

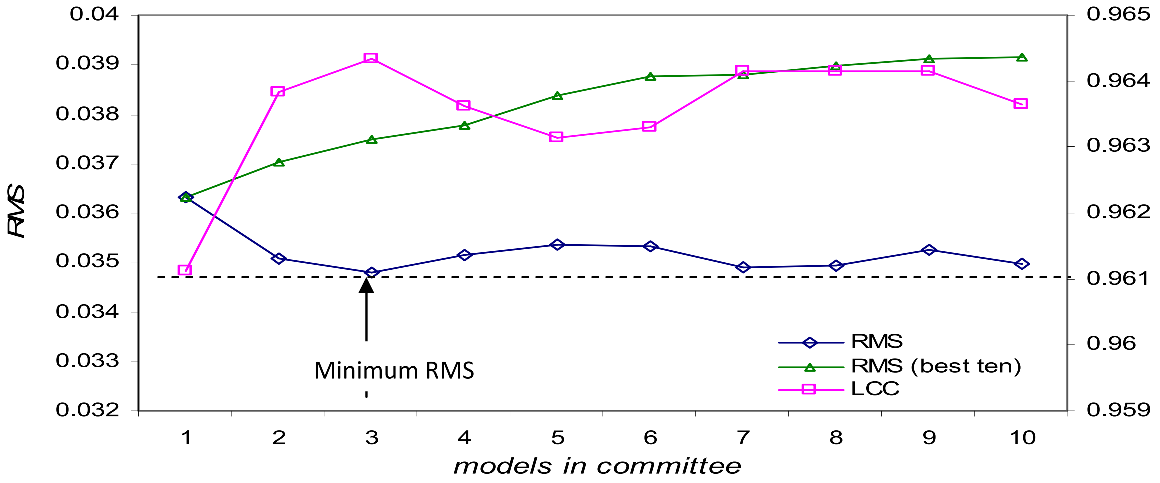

Figure1- Effect of averaging process on Yield Strength model.

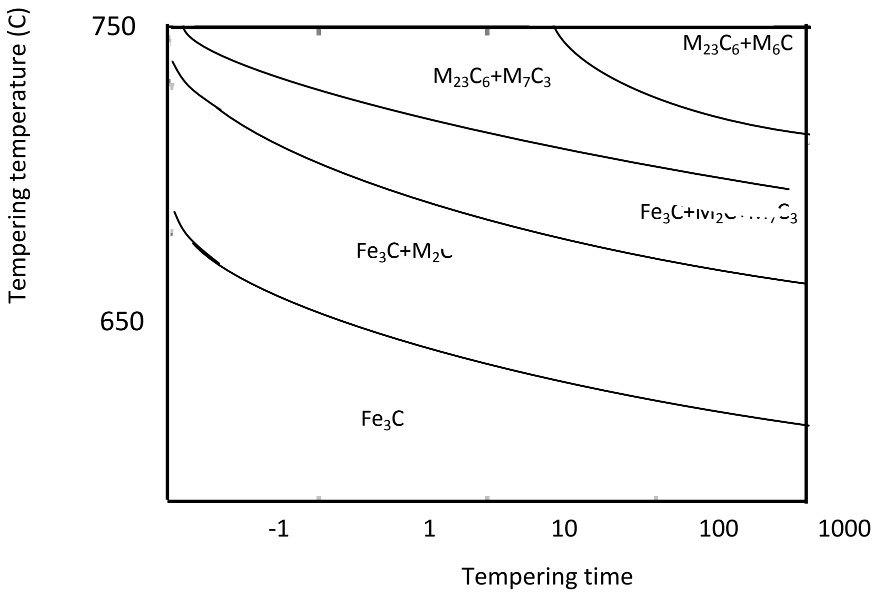

Figure 2- Tempered martensite carbides transformation sequence in 2¼Cr-1Mo steel [Bhadeshia, H. K. D. H., 1999].

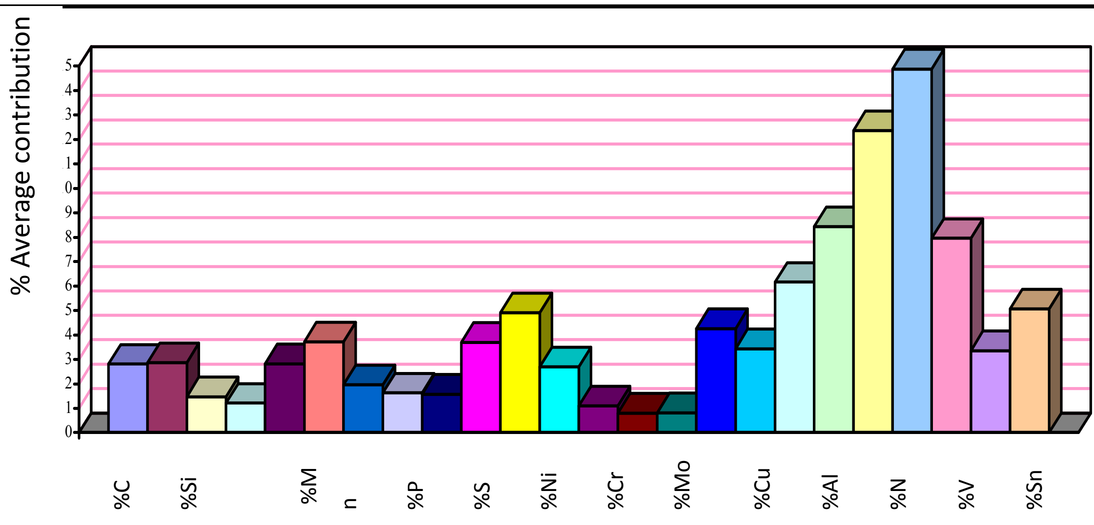

Figure 3- A histogram showing contributions of input nodes on YS model.

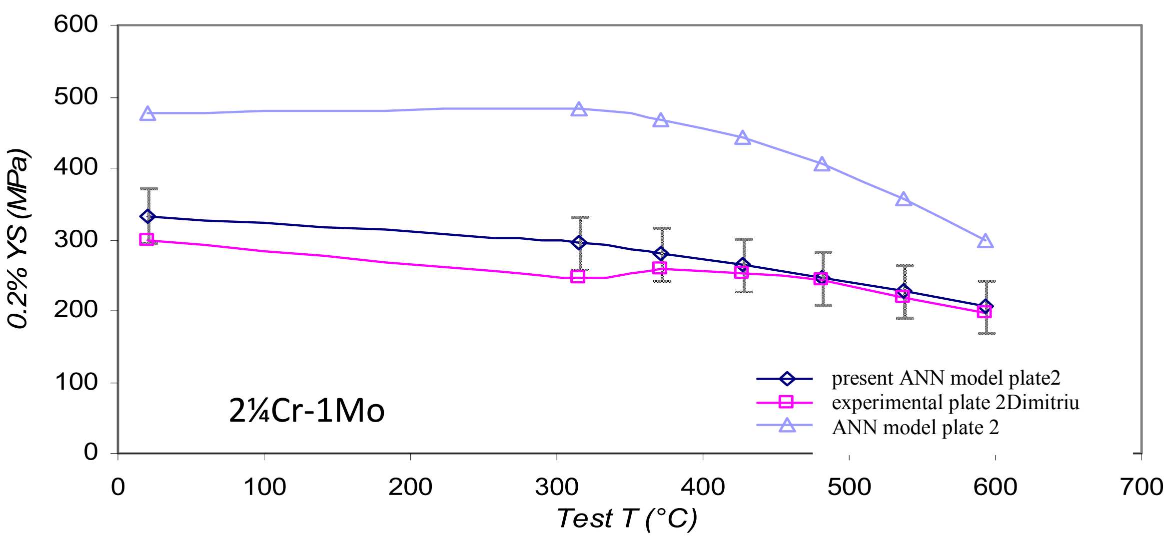

Figure 4- Comparison between predicted and true (experimental data) YS.

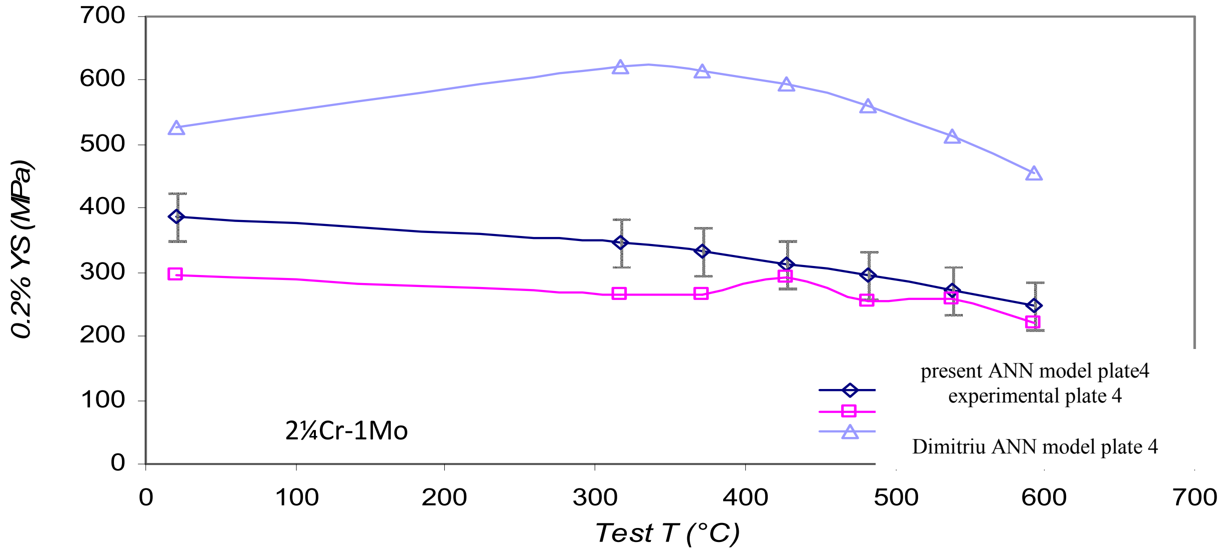

Figure 5- Comparison between predicted and true (experimental data) YS.

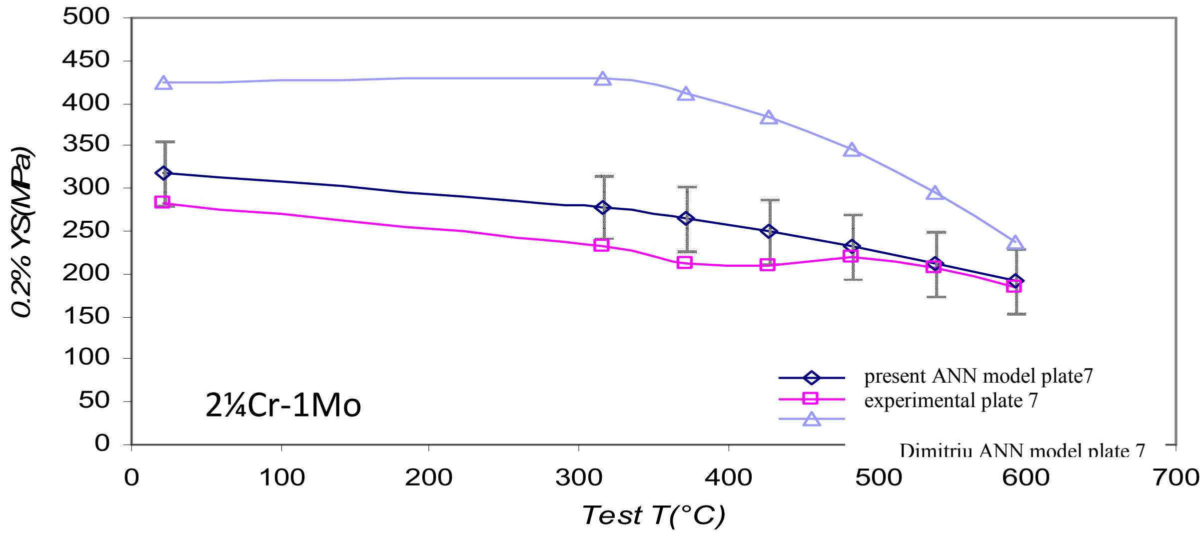

Figure 6- Comparison between predicted and true (experimental data) YS.

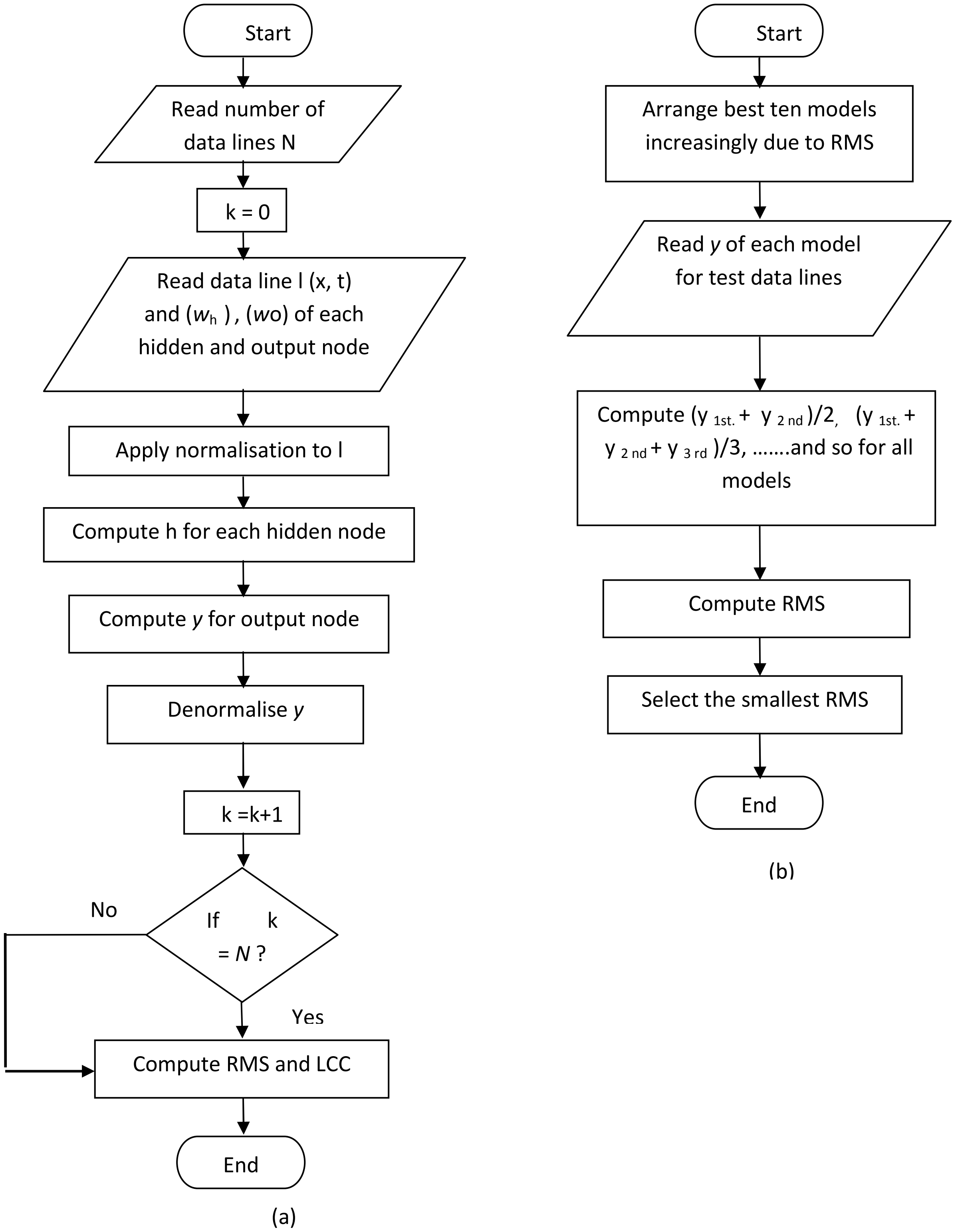

Figure 7- Flow charts of programs used in the present work: (a) Neural networks computation flow chart and (b) Models in committee flow chart (averaging).

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Nomenclature

ANN: artificial neural networks.

%EL : elongation.

K : Constant (0, 1,…, N).

L : Data line l (x ; t).

LCC : linear correlation coefficient.

M : alloying element forming carbides.

N : Number of data lines.

%RA: reduction of area.

RMS: root mean square value error.

t : Target value (strength from data).

TS : tensile strength.

$w_0, \ldots w_h$: Weights of the hidden and output layers (parameter value).

y : predicted value of strength.

YS : yield strength.