MODELING MECHANICAL PROPERTIES OF STEELS BY MEANS OF NEURAL NETWORKS

Renata Neves Penha, rnp@usp.br
Lauralice Franceschini Canale, lfcanale@sc.usp.br
Departamento de Engenharia de Materiais, Aeronáutica e Automobilistica – EESC-USP
Av. Trabalhador São-carlense, 400, Centro. 13566-590. São Carlos - SP

Abstract. *Neural networks represent a more general regression method, which gives better results than linear regressions. It is a powerful tool especially for problems that do not have a completely accepted physical model, such as many problems encountered in materials sciences. The tempering process aims to get the microstructures that lead to service mechanical properties and, to promote the relaxation of the residual stresses generated during quenching. The goal of this work is to predict the effect of tempering time and temperature on some steels properties by means of neural networks. Five types of steels, AISI 5160, AISI 6150, AISI E52100, AISI 4140 and AISI 4340, were tempered in different conditions. The inputs of the neural network are the chemical composition and the tempering time and temperature; the outputs are the tensile strength, the rupture stress, the modulus of elasticity and the hardness.*

Keywords*: tempering, neural networks, mechanical properties.*

1. INTRODUCTION

During tempering of quenched steels, changes on microstructure are produced over a wide range, resulting in corresponding changes in mechanical properties. The tempering process is dependent of the relation time-temperature. The selection of these process parameters affects temper embrittlement, non-optimal stress relief, hardness, tensile strength, yield strength and transformation of retained austenite.

This relation has been already reported by Hollomon and Jaffe (1945), when they noticed that the same hardness could be reached by different time-temperature histories. In this work they have obtained a relation between hardness (H) and a tempering parameter (c), as follows on Eq.(1):

$$f(H)=f[T(c+logt)] \tag{1}$$

As they had worked only with plain carbon steels, many authors had suggested that this model do not fit well all types of steel, a review of the development of the tempering parameters development has been reported by Canale, et.al. (2006). Grange and Baughman (1956) suggested C=18 for all carbon steels. Nehrenberg (1950) used C=20, and developed tempering curves for a series of stainless steels. An example of the use of neural networks to the same proposal was made by Filetin et al. (1999), but their work has focused only on tempering curves, namely hardness of tool steels. The aim of this work is to calculate hardness, tensile strength, rupture stress and the Young's modulus for five alloyed steels, tempered in different conditions of time and temperature by means a simple neural network.

Heat treatment of materials is a fundamental metallurgical process, which involves very complex and nonlinear phenomena. In this way, physical models are difficult or impossible to obtain. In such cases neural networks seems to be a powerful tool. Mackay (1997) has defined neural networks as a general method of regression analysis in which a flexible non-linear function is fitted to experimental data.

2. EXPERIMENTAL PROCEDURE

The samples were austenitized at 850ºC, and quenched in a mineral oil. Figure 1 shows the specimen, which one were machined following the ASTM E8M Standard (tensile testing). Three specimens were tempered at specified time and temperature, and cooled in air. The selected temperatures were 100, 150, 200, 250, 300, 400, 500, 600 and 700ºC. During tempering process the furnace temperature varied ±10ºC. The time on each temperature was 10s, 90s, 900s, 9000s and 86400s. According to ASTM E8M Standard each condition test must have reproducibility equal 3, so there were tested 675 samples. Table 1 shows the chemical composition of five types of steel used in this work.

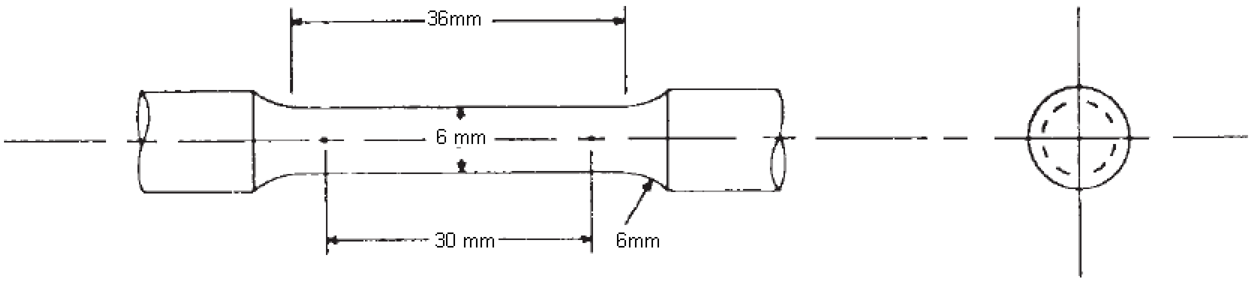

Figure 1: Specimen following the ASTM E8M standard for tensile testing.

Table 1: Chemical Composition of tested steel.

Steel	%C	%Mn	%P	%S	%Si	%Ni	%Cr	%Mo
AISI 4140	0.41	0.88	0.016	0.018	0.23	-	1.02	0.22
AISI 4340	0.39	0.75	0.019	0.016	0.26	1.74	0.79	0.26
AISI 5160	0.62	0.88	0.012	0.018	0.22	-	0.79	-
AISI 6150	0.51	0.81	0.021	0.014	0.28	-	0.98	-
AISI E 52100	1.02	0.40	0.017	0.014	0.23	-	1.42	-

After quenching and tempering the samples was submitted to tensile test performed in a universal MTS machine with a load of 100KN and extensometer of 25mm. The strain rate was set to 0.8 mm/min. So it was measured the superficial hardness in the head of each specimen. Five hardness measurements were collected using a LECO RT-240 durometer, with a load of 150kgf. As it was obtained a large amount of data it were decided to present here only the results used o test the neural network either for tensile test as for hardness. Figures 2 to 6 show the stress-strain curves obtained for ten conditions picked out randomly of the set. Figure 2 (a) shows the stress-strain (σ-ε) curve obtained for the AISI 4140 steel tempered for 9000s at 250ºC, while Fig. 2 (b) shows the curve for the same steel tempered for 10s at 700ºC. In common sense lower time on temperature should provide a curve with a brittle behavior, but as it can be seen in this figure at higher temperatures it is not the rule.

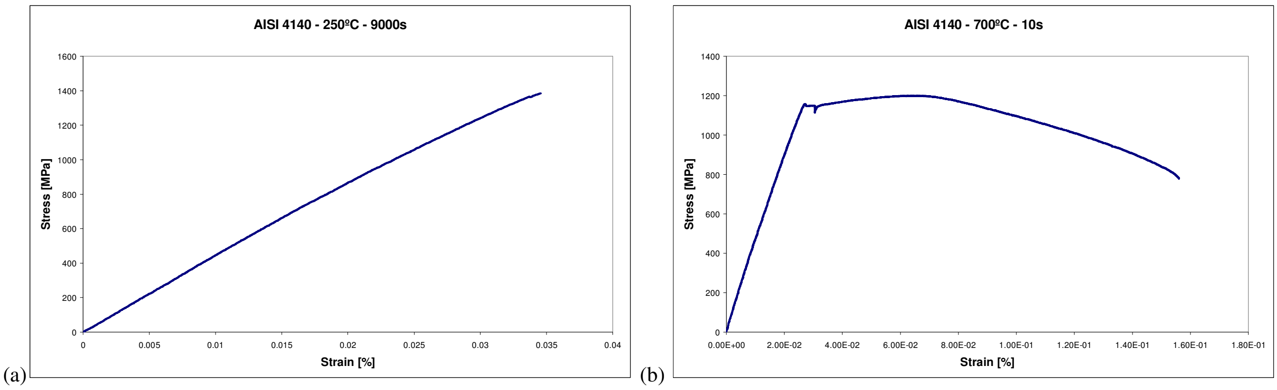

Figure 2: Stress-strain curve for AISI 4140 steel tempered for (a) 9000s at 250ºC and (b) 10s at 700ºC.

Figure 3 shows the stress-strain curves obtained for AISI 4340 steel that was heat treated for 900s at 300ºC (Fig. 3 (a)) and for 90s at 400ºC (Fig. 3 (b)). In Fig. 4 (a) it can be observed the tensile curve for an AISI 5160 tempered for 86400s at 100ºC, and Fig. 4 (b) 900s at 400ºC. The data obtained for AISI 6150 steel is showed by Figure 5 (a) 9000s at 150ºC, and Figure 5 (b) 90s at 500ºC. Figure 6 shows the curves picked out for the AISI E52100 steel, tempered for 56400s at 200ºC, Fig. 6 (a), and for 10s at 600ºC on Fig. 6 (b). Table 2 shows the mean superficial hardness of the five measurements for the test set.

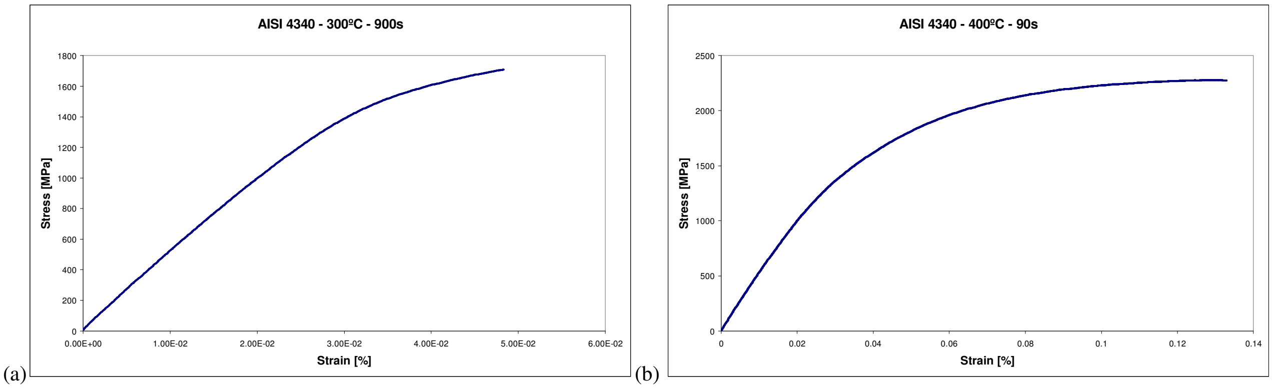

Figure 3: Stress-strain curve for AISI 4340 steel tempered for (a) 900s at 300ºC and (b) 90s at 400ºC.

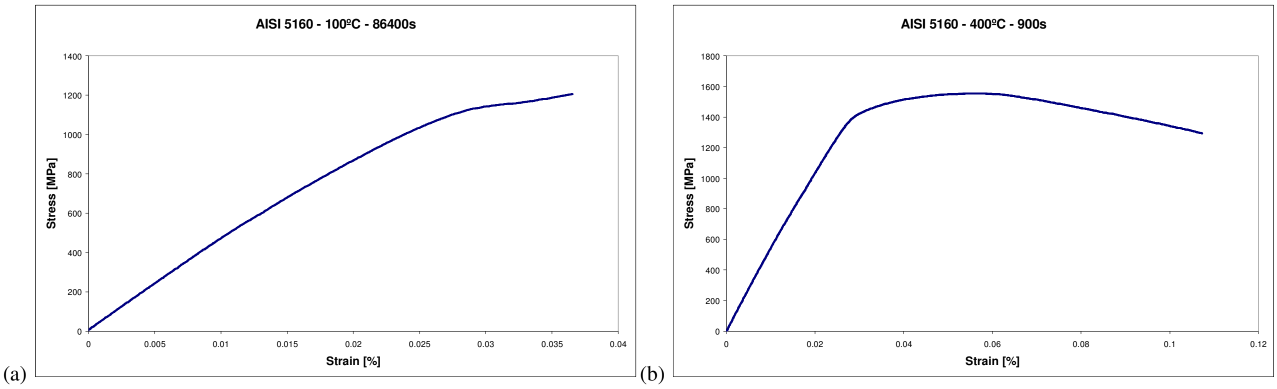

Figure 4: Stress-strain curve for AISI 5160 steel tempered for (a) 86400s at 100ºC and (b) 300s at 400ºC.

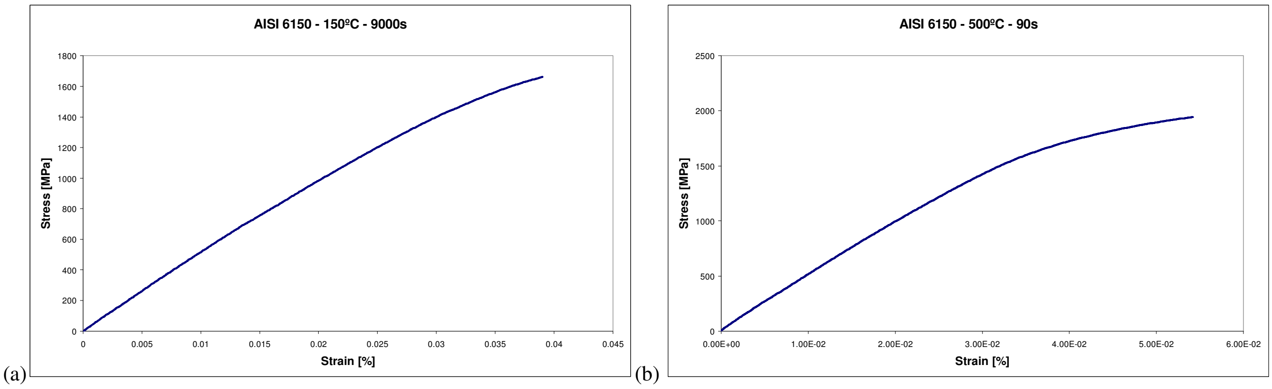

Figure 5: Stress-strain curve for AISI 6150 steel tempered for (a) 9000s at 150ºC and (b) 90s at 500ºC.

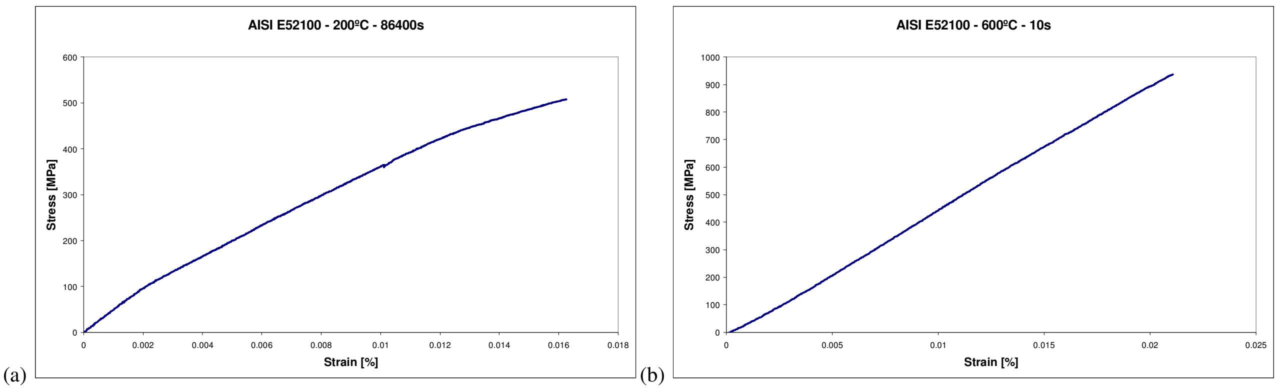

Figure 6: Stress-strain curve for AISI E52100 steel tempered for (a) 86400s at 200ºC and (b) 10s at 600ºC.

Table 2: Superficial hardness for test set.

Steel	Tempering Condition	Hardness [HRc]
AISI 4140	9000s at 250ºC	57.0
	10s at 700ºC	49.8
AISI 4340	900s at 300ºC	54.9
	90s at 400ºC	48.6
AISI 5160	86400s at 100ºC	56.4
	900s at 400ºC	43.0
AISI 6150	9000s at 150ºC	49.1
	90s at 500ºC	42.9
AISI E52100	86400s at 200ºC	49.9
	10s at 600ºC	51.2

3.NEURAL NETWORKS

Four feed forward networks were built with chemical composition, tempering temperature and time on temperature as inputs and, tensile strength, rupture stress, modulus of elasticity and hardness as outputs of each neural network. It was decided to work with one network for each output due to small amount of data available, so that it would be possible to reduce the number of free parameters and improve generalization. The activation function was set as a tangent hyperbolic function as shown in Eq. (2) in the hidden layers, while a linear function was used for the output layer as shown in Eq. (3):

$$h_i = \tanh\left(\sum w_{ij} x_j + \theta_i\right) \tag{2}$$

$$y = \sum w_i h_j + \theta_i \tag{3}$$

where x_j are the inputs and w_{ij} are the weights, which define the neural network. The biases θ_i are treated internally as weights associated with a constant input set to unity.

To train the neural network was used the MATLAB function *traingdm*, which combines adaptive learning rate with momentum training. The initial learning rate was set at 0.01 and the momentum at 0.9. The network was trained until 15000 epochs. Many network architectures were tested until to find the best configuration. It was verified that a neural network with two hidden layers with six and ten neurons respectively, was that one that promoted the best fit for the output layer. Each neural network had 10 inputs and just one output. The range, mean and standard deviation of input data are listed on Table 3.

Table3: Input data.

Input variables	Min.	Max.	Mean	Standard deviation
Temperature [ºC]	99	703	382.7	196.3
Time [s]	10	86400	20075	33684
%C	0.39	1.02	0.597	0.232
%Mn	0.4	0.88	0.739	0.180
%P	0.012	0.021	0.017	0.003
%S	0.014	0.018	0.016	0.002
%Si	0.22	0.28	0.244	0.023
%Ni	0	1.74	0.361	0.707
%Cr	0.79	1.42	0.99	0.235
%Mo	0	0.26	0.0914	0.118

To avoid the overfitting problem the Bayesian regularization was used. This method consists in modifying the performance function, Eq. (4), which is normally chosen to be the sum of squares of the network errors on the training set. The function is modified by adding a term (Eq. (5)) that consists of the mean of the sum of squares of the network weights (*msw*) and biases in the original function. It causes the network to have smaller weights and biases and, this forces the network response to be smoother and less likely to overfit. The new performance equation corresponds to Eq. (6).

$$mse = \frac{1}{N}\sum_{i=1}^{N}(t_i - a_i)^2 \tag{4}$$

$$msw = \frac{1}{N}\sum_{j=1}^{N}w_j^2 \tag{5}$$

$$msereg = \gamma mse + (1-\gamma)msw \tag{6}$$

where N is the number of samples, t the desired output, a the value calculated by the neural network and γ the performance ratio.

The data set was obtained experimentally as shown on section 2. It was divided between training set and test set. The training set was composed of 225 conditions and the test set of 10 conditions picked out randomly from training set.

4. RESULTS AND DISCUSSION

After the training section the final error obtained by the modified performance function, given by Eq. (6), was equal to 0.209, 0.221, 0.434 and 0.067 for tensile strength, rupture stress, modulus of elasticity and hardness. Figure 7 shows the measured and calculated tensile strength obtained for training and test data set. To evaluate this neural network there were calculated the correlation coefficient (R value), a straight line and the equation obtained for the best linear fit for the data. As it is illustrated on Fig. 7, tensile strength was well adjusted by the neural network. Rupture stress (Fig. 8) displays a similar behavior of tensile strength.

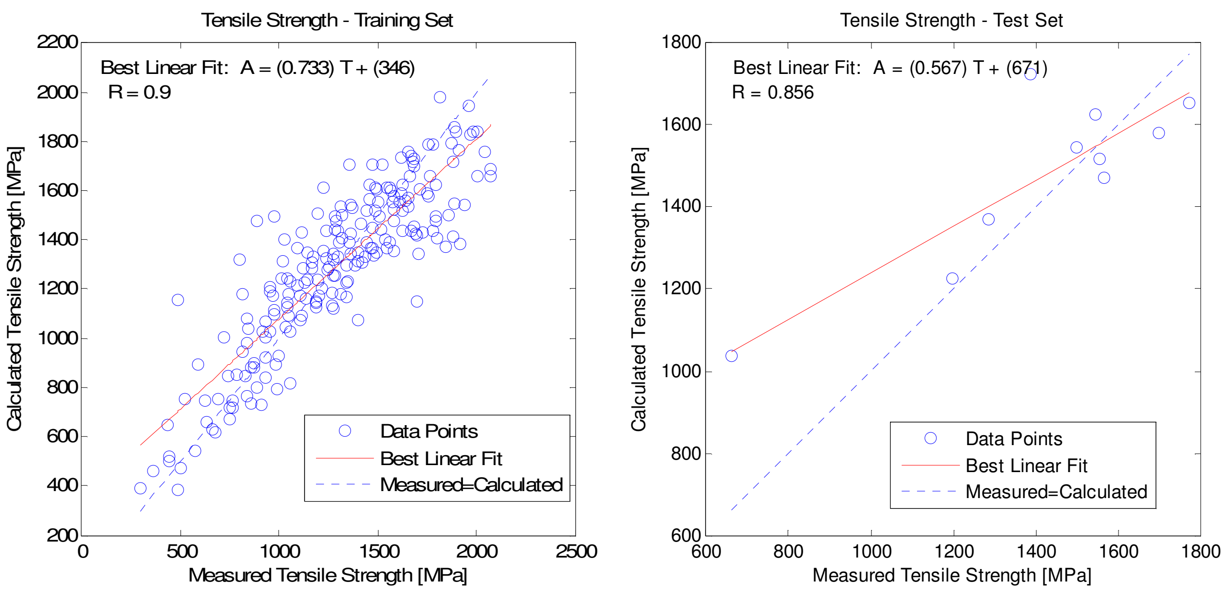

Figure 7: Predicted tensile strength by the neural network versus experimental values for (a) training and (b) test data sets.

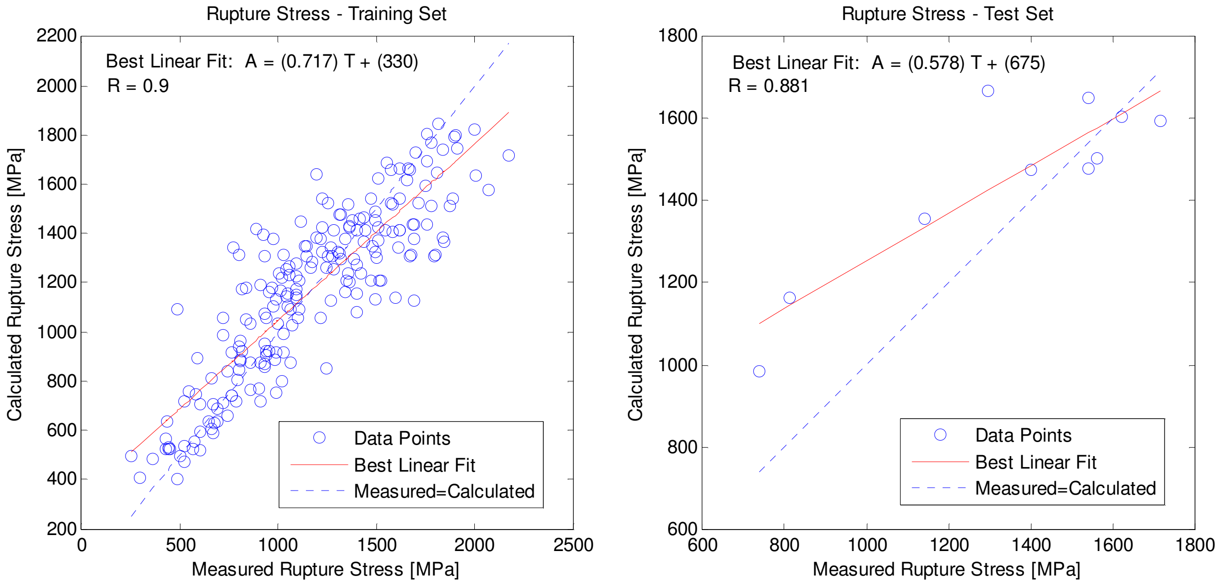

Figure 8: Predicted rupture stress by the neural network versus experimental values for (a) training and (b) test data sets.

Figure 9 compares the experimental values and the calculated values obtained for the elastic modulus. In this case the architecture did not adjust the data adequately. A probable reason for that could be the amount of data that was not sufficient in this case. The final value given by the performance function was equal to 0.434, higher than all others cases.

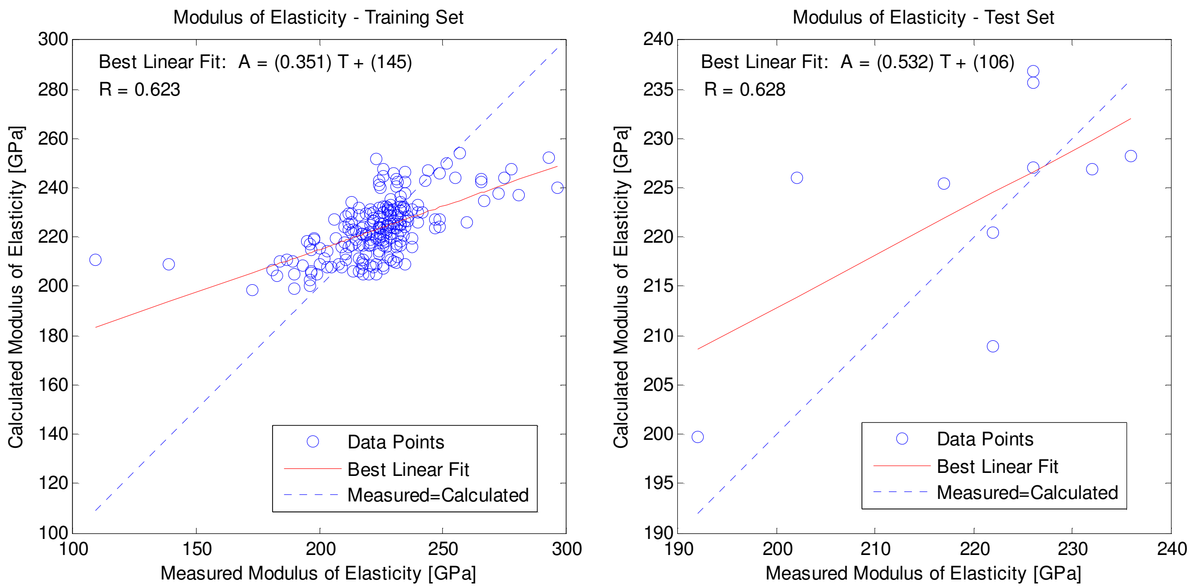

Figure 9: Predicted modulus of elasticity by the neural network versus experimental values for (a) training and (b) test data sets.

Hardness results can be seen in Fig. 10. In this case the neural network fitted well training and test data sets. The neural network made to calculate hardness was that with lower value for performance function.

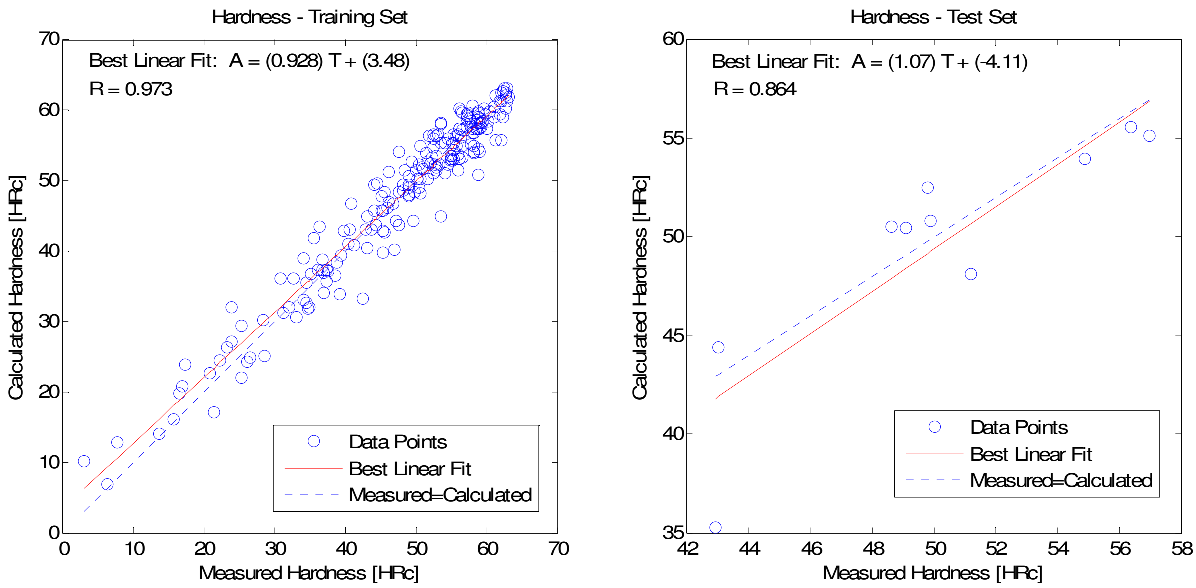

Figure 10: Predicted hardness by the neural network versus experimental values for (a) training and (b) test data sets.

5. CONCLUSIONS

As can be verified neural networks are a powerful tool to predict mechanical properties of steels. Generally these networks are constructed just for one type of steel. This work was an attempt to model five types of steel, and results obtained in here encourage more investigations in this area. It could be tested others types of neural networks, such as radial bases or wavelets neural networks, these networks generates less free parameters so it would not be necessary to enlarge the amount of data set. Another way to improve this generalization could be enlarging the data set. The great potential of using neural networks is the economic benefits that it can provide for the industry, because it can reduce the necessity of expensive experimental investigation of steels and its mechanical properties.

6. ACKNOWLEDGEMENTS

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