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ORIGINAL ARTICLE

Predictions of toughness and hardness by using chemical composition and tensile properties in microalloyed line pipe steels

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Abstract Artificial neural networks with multilayer feed forward topology and back propagation algorithm containing two hidden layers are implemented to predict the effect of chemical composition and tensile properties on the both impact toughness and hardness of microalloyed API X70 line pipe steels. The chemical compositions in the forms of "carbon equivalent based on the International Institute of Welding equation (CE_{IIW})", "carbon equivalent based on the Ito-Bessyo equation (CE_{Pcm})", "the sum of niobium, vanadium and titanium concentrations (VTiNb)", "the sum of niobium and vanadium concentrations (NbV)" and "the sum of chromium, molybdenum, nickel and copper concentrations (CrMoNiCu)", as well as, tensile properties of "yield strength (YS)", "ultimate tensile strength (UTS)" and "elongation (El)" are considered together as input parameters of networks while Vickers microhardness with 10 kgf applied load (HV10) and Charpy impact energy at −10 °C (CVN −10 °C) are assumed as the outputs of constructed models. For the purpose of constructing the models, 104 different measurements are performed and gathered data from examinations are randomly divided into training, testing and validating sets. Scatter plots and statistical criteria of "absolute fraction of variance (R^2)", and "mean relative error (MRE)" are used to evaluate the prediction performance and universality of the developed models. Based on analyses, the proposed models can be further used in practical applications and thermo-mechanical manufacturing processes of microalloyed steels.

Keywords Artificial neural network (ANN) · Chemical composition · Microalloyed steel · Line pipe steel · Toughness · Hardness

1 Introduction

The high strength low alloy (HSLA) steels are developed by combining the benefits of the precipitation hardening of microalloying elements along with the advantages of the grain refinement. Controlled rolling and accelerated cooling are the two major processing routes of HSLA steels. A complex chemistry, as well as, complicated thermo-mechanical processing history has led to the introduction of some advanced steels in this grade. The microalloyed and/or HSLA steels are widely used in the construction of high pressure gas transportation line pipes. High strength levels together with excellent toughness and good weldability are the main characteristics and requirements of these steels [1–3]. The required standards for their use in conveying gas and petroleum in both oil and natural gas industries are provided by American Petroleum Institute (API). According to API 5L [4] and ISO 3183 [5] standards, strength of these steels is evaluated by tensile testing while drop weight tear testing and Charpy V-notch impact testing are used for assessment of their toughness. Also, alloy design with regard to the upper limit of equivalent carbon content is specified by the above standards; however, in turn they guarantee the good weldability of such pipes [4]. Different grades of API steels are currently in use and utilization of higher grades containing API X100 and API X120 as the

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next generations of line pipe steels are under consideration [6–8].

In manufacturing processes of these grades of steels, chemical composition and thermo-mechanical control process (TMCP) schedule are the most important decision-making areas that influence their final microstructure and mechanical properties [1–3, 6]. Generally, microstructure of these steels for the lower grades up to API X65 is ferritic–pearlitic since for the higher grades (API X70 and X80) is acicular ferritic–bainitic [9, 10]. The API X70 can be produced either in ferritic–pearlitic or acicular ferritic–bainitic microstructure [11, 12]. Also, a predominantly bainitic microstructure has been reported for a typical API X100 steel [6, 13].

In line pipe steels, chemical composition with low C content (<0.1 wt%) and high Mn content (1.4–1.9 wt%) results in a good combination of weldability, toughness and strength [10, 12]. Mo, Cu and Ni are added to improve the strength. Additions of microalloying elements such as Nb, Ti, V and Al form carbides, nitrides and carbonitrides and also lead to grain refining and precipitation strengthening. Fine TiN precipitates will be stable up to high temperatures and prevent the excessive grain growth of austenite during reheating [10, 14]. Nb is the most important microalloying element. Nb(C, N) at higher temperatures, reheating temperature for instance, will be in solid solution. Precipitations of Nb(C, N) at higher rolling temperatures under deformation condition (strain induced precipitation) prevent grain growth during rough rolling and recrystallization of austenite at final rolling stage. The latter is the highlighted role of Nb in austenite pancaking [15]. Meanwhile, Nb in solid solution retards the recrystallization and increases non-recrystallization temperature (T_{nr}) [16]. This allows conducting the final rolling stage of TMCP at higher temperature with lower rolling force. During accelerated cooling, further precipitation of the remaining Nb in the form of fine particles enhances its strengthening effect [17]. As V is in solid solution at temperatures above 1,000 °C; it plays an important role during accelerated cooling in precipitation strengthening of ferrite [10, 18]. With regard to the upper limits specified by API 5L standard, S and P should be kept in possible lower contents ($P < 0.030$, $S < 0.030$) [4].

The prediction of mechanical properties of microalloyed steels is a sophisticated task and needs an in depth knowledge of the whole processing parameters. Recently, artificial neural networks (ANNs) have been widely used for investigating the correlation between final mechanical properties and the chemical composition and/or processing parameters of different steels [19–23]. The aim of the present study was to develop ANN-based models to predict the effects of chemical composition, as well as, tensile parameters on the hardness and impact properties of microalloyed API X70 line pipe steels.

2 Experimental procedure

The room temperature tension test samples are machined based on the ASTM E8M standard [24] with consideration that the pipe body area which tension samples are cut from would be in accordance to the API 5L standard [4]. The specimen gauge length is kept 50.8 mm which is utilized to measure the specimens' extension. Also, the impact test samples with dimensions of 10 mm × 10 mm × 55 mm are cut transverse to the rolling axis from the body of pipes in accordance to the API 5L standard. Then, all machined and prepared according to the ASTM E23M standard dimensions [25]. During the test, samples are struck with a high-energy pendulum (750 J) at −10 °C. According to the API 5L and ISO 3183 standards, the minimum average (of a set of three test coupons) absorbed energy for each pipe body shall be based upon the full-size test coupon at test temperature of 0 °C and/or if agreed, at a lower test temperature might be selected. It is revealed that microalloyed steels usually have high absorbed energy in impact testing since their ductile-to-brittle transition temperatures are below −70 °C.

The Vickers microhardness measurement load is maintained 10 kgf while the dwelling time is kept 15 s throughout examinations. The transverse hardness samples are prepared according to IPS standard [26]. Steels' chemical analyses of elements are carried out using ARL 2460 quantometer. Sample preparation and tests are performed according to the ASTM A751 standard [27], and specimens are extracted from the body of pipes.

In the present study, the ANN-based models have been trained, tested and validated for predicting the impact toughness and hardness of X70 microalloyed steels. For this purpose, the experimental data of 104 line pipe steels from several suppliers having different chemical compositions have been utilized. The input variables of ANN modelings are comprised of weight percentage of alloying elements and tensile properties of steels. Chemical compositions in the form of 5 different variables and tensile characteristics in the form of three different variables totally making 8 inputs are considered in modelings. Table 1 summarizes the input and output parameters along with their statistics. Meanwhile, supplementary details on the input and output data characteristics are presented in Figs. 1, 2 and 3. For categorization of gathered data in above figures, standard deviation is considered as the

Table 1 Input and output parameters along with their statistics used in the ANN-based modelings

Parameter	Unit	Minimum	Maximum	Average	Standard deviation	Median	Variance
Input							
CE_{IIW}	wt%	0.35483	0.39635	0.37587	0.00848	0.37401	0.00007
CE_{Pcm}	wt%	0.15404	0.18937	0.17197	0.00769	0.17102	0.00006
VTiNb	wt%	0.04433	0.05499	0.04974	0.00221	0.04972	0.00000
CrMoNiCu	wt%	0.37588	0.46894	0.40895	0.02233	0.40518	0.00050
NbV	wt%	0.03349	0.04196	0.03795	0.00158	0.03796	0.00001
YS	MPa	462.99	570.78	521.78	22.71	–	–
UTS	MPa	567.90	684.79	619.29	18.77	–	–
El	%	32.00	41.00	35.35	1.82	35.00	3.30
Output							
CVN (−10 °C)	J	222.00	353.00	290.16	29.03	290.00	842.78
HV10	kgf	192.00	224.00	204.93	6.89	204.00	47.46

criterion. Also, Fig. 4 illustrates the general bimodal ferritic–pearlitic microstructure of API X70 steels by the both optical and scanning electron microscopy techniques.

Considering the API 5L standard, the values for inputs are comprised of "carbon equivalent based on the International Institute of Welding equation (CE_{IIW}) [28] (Eq. 1)", "the carbon equivalent based on the Ito-Bessyo carbon equivalent equation (CE_{Pcm}) [29] (Eq. 2)", "the sum of the niobium, vanadium and titanium concentrations (VTiNb)", "the sum of the niobium and vanadium concentrations (NbV)", "the sum of the chromium, molybdenum, nickel and copper concentrations (CrMoNiCu)", "the yield strength at 0.005 offset (YS)", "ultimate tensile stress (UTS)" and "percent elongation (El)". The values for the output are selected as "Charpy impact test at −10 °C (CVN −10 °C)" and "Vickers microhardness using 10 kgf load (HV10)".

$$CE_{IIW} = C + \frac{Mn}{6} + \frac{(Cr + Mo + V)}{5} + \frac{(Ni + Cu)}{15} \quad (1)$$

$$CE_{Pcm} = C + \frac{Si}{30} + \frac{(Mn + Cu + Cr)}{20} + \frac{Ni}{60} + \frac{Mo}{15} + \frac{V}{10} + 5B \quad (2)$$

3 Results and discussion

Four-layer feed forward ANNs with back propagation algorithms are implemented to predict the toughness and hardness of line pipe steels. This neural network modeling has a powerful input–output mapping capability. With the use of enough hidden neurons, it can effectively approximate any continuous nonlinear function [30]. In the proposed models, one input layer, two hidden layers with hyperbolic sigmoid activation function, as well as, one output layer with linear activation function is used. In feed forward neural networks, weights and biases are adjusted iteratively to minimize the network performance function by using a training algorithm. The commonly used performance function in these neural networks is mean square error (MSE) [31]:

$$MSE\ (\%) = \frac{1}{n}\sum_{i=1}^{n} (t_i - o_i)^2 \times 100 \quad (3)$$

where t_i is the measured (actual) value of ith data, o_i is the predicted value for ith data as output variable, and n is the total number of variables. Here, Bayesian regularization training algorithm is used to train the networks. In this training algorithm, weights and biases are updated with Levenberg–Marquardt optimization algorithm. The network generalization improves by minimizing the combination of MSE and the mean square of the network weights. Also, the weights are considered as random variables with Gaussian distribution. To improve the generalization property of the proposed models, the early stopping technique is used and the overall data are randomly divided into three subsets of training, testing and validating. In this technique, training process should be stopped when the error for the validation set starts to increase. The error value of testing demonstrates if the overfitting has been occurred. As it is summarized in Table 1, the collected experimental data included 104 patterns of which 74 patterns are used for training the network. The remained data are divided equally into two subsets containing 15 data sets to validate and test the trained networks.

The numbers of nodes in the all layers are equal to the number of inputs and outputs of the networks, i.e., 8 and 1 for the present work, respectively. The number of nodes in the hidden layers is obtained through trial and error during training and testing processes of the networks. Usually, scatter diagrams are used to plot the predicted values of the networks versus measured (experimental) ones. In this research, in addition to the scatter plots, two statistical

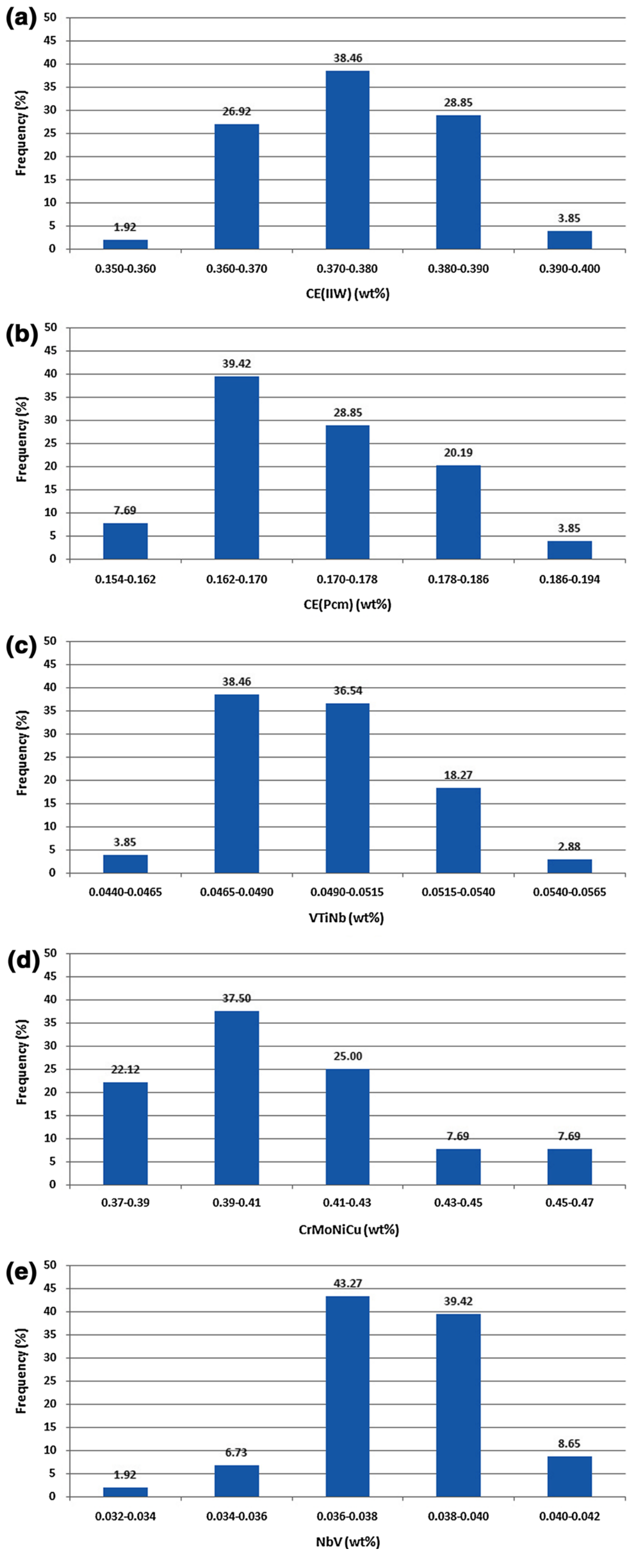

Fig. 1 Repetition frequency of chemical compositions as modeling inputs extracted from examinations: **a** CE_{IIW}, **b** CE_{Pcm}, **c** VTiNb, **d** CrMoNiCu and **e** NbV

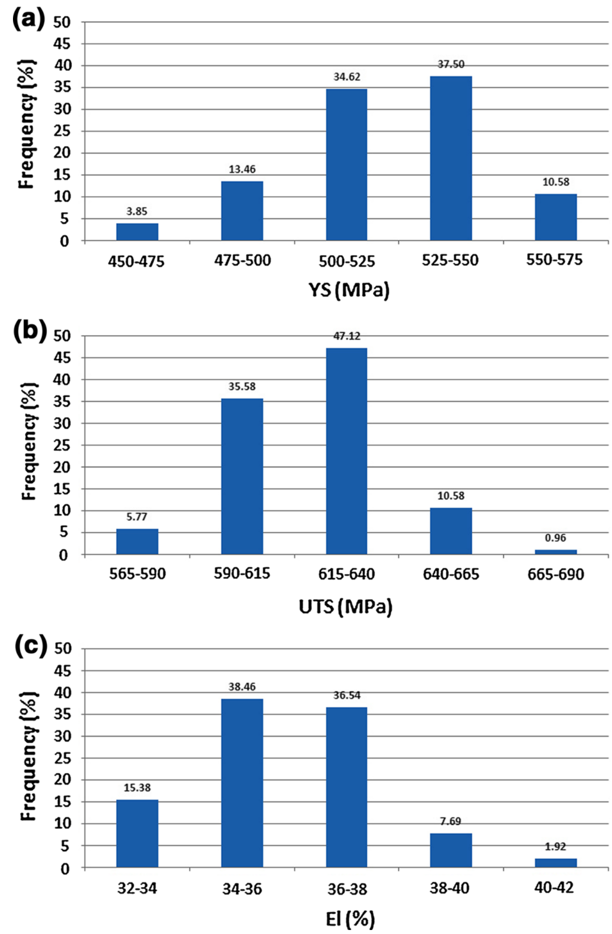

Fig. 2 Repetition frequency of tensile characteristics as modeling inputs extracted from examinations: **a** yield strength, **b** ultimate tensile strength and **c** elongation

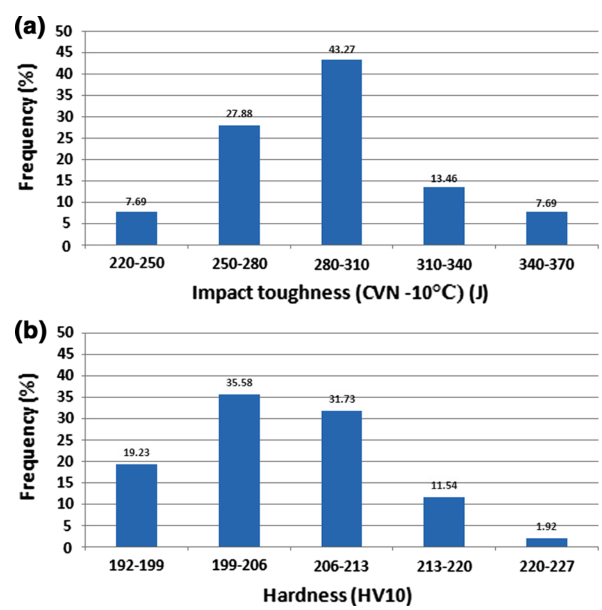

Fig. 3 Repetition frequency of **a** impact toughness and **b** hardness in examinations

criteria, i.e., absolute fraction of variance (R^2) and mean relative error (MRE), are used to evaluate the predicting precision of the proposed models as follows [32]:

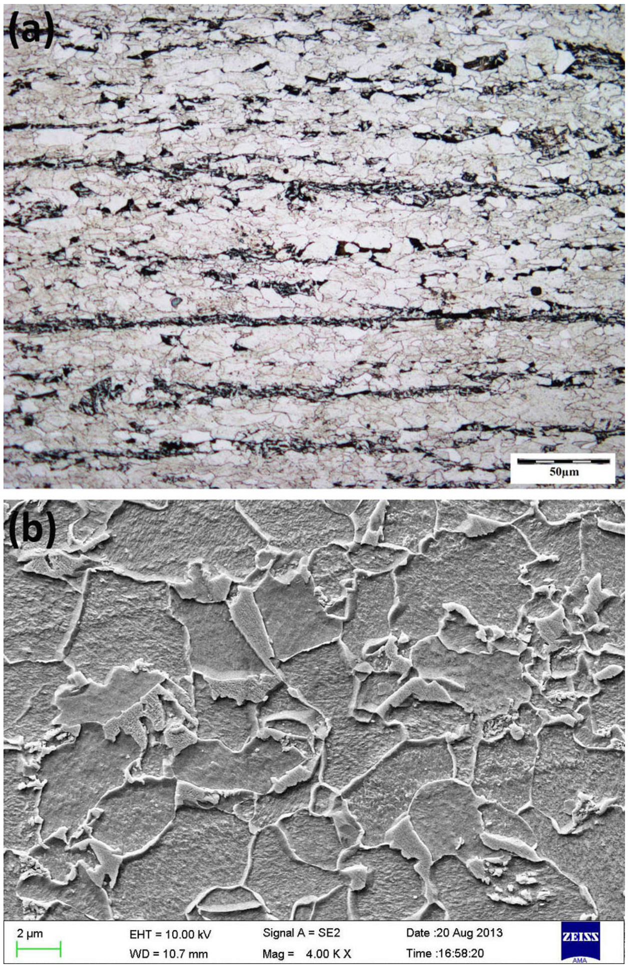

Fig. 4 Bimodal ferritic–pearlitic microstructure of API X70 micro-alloyed steels acquired by **a** optical and **b** scanning electron microscope

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{n} (t_i - o_i)^2}{\sum_{i=1}^{n} (o_i)^2} \right) \tag{4}$$

$$\mathrm{MRE}\ (\%) = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{t_i - o_i}{t_i} \right| \times 100 \tag{5}$$

where t_i, o_i and n are defined in Eq. 3. The reliability and robustness of a neural network depends on many parameters including learning constants, activation function and random distribution of the weights in the initiation of training process along with the number of nodes in the hidden layers. The small number of nodes in the hidden layers leads to underfitting since the high number causes overfitting. Numbers of neural networks with 12–36 nodes in their hidden layers are trained, and the MRE values for training and testing datasets of networks are extracted and calculated. It is determined that the network with 20 nodes in the first hidden layer and 12 nodes in the second hidden layer had the less MRE value for the testing data. The increase in the number of these nodes did not improve the network results for training data. So, the networks' structures in the present study are considered 8-20-12-1 representing inputs nodes in the first hidden layer-nodes in second hidden layer-target.

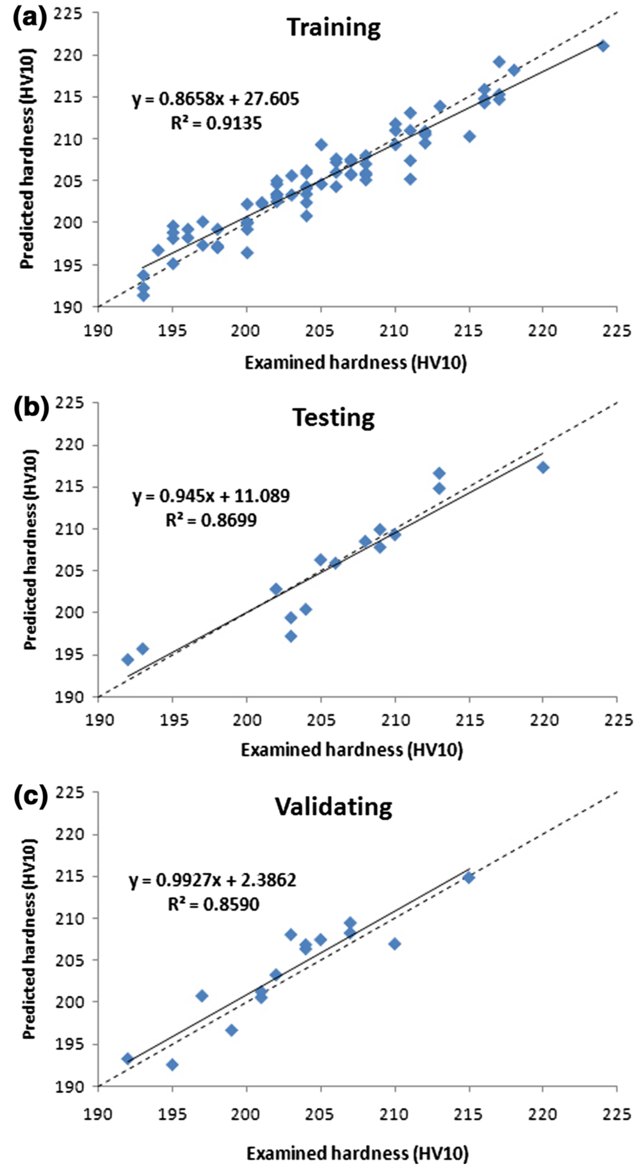

Fig. 5 The correlation of examined and predicted hardness values in **a** training, **b** testing, and **c** validating datasets through ANN-based model

The results of the developed ANN models to predict the toughness and hardness of steels in the form of scatter plots and calculated R^2 values are shown in Figs. 5 and 6, respectively. Also, the calculated MRE values for overall data and training, testing and validating subsets are presented in Table 2. As it can be seen from Figs. 5, 6 and Table 2, the developed feed forward ANN-based models with R^2 upper than of 0.86 and mean relative error lower than 2.11 % for

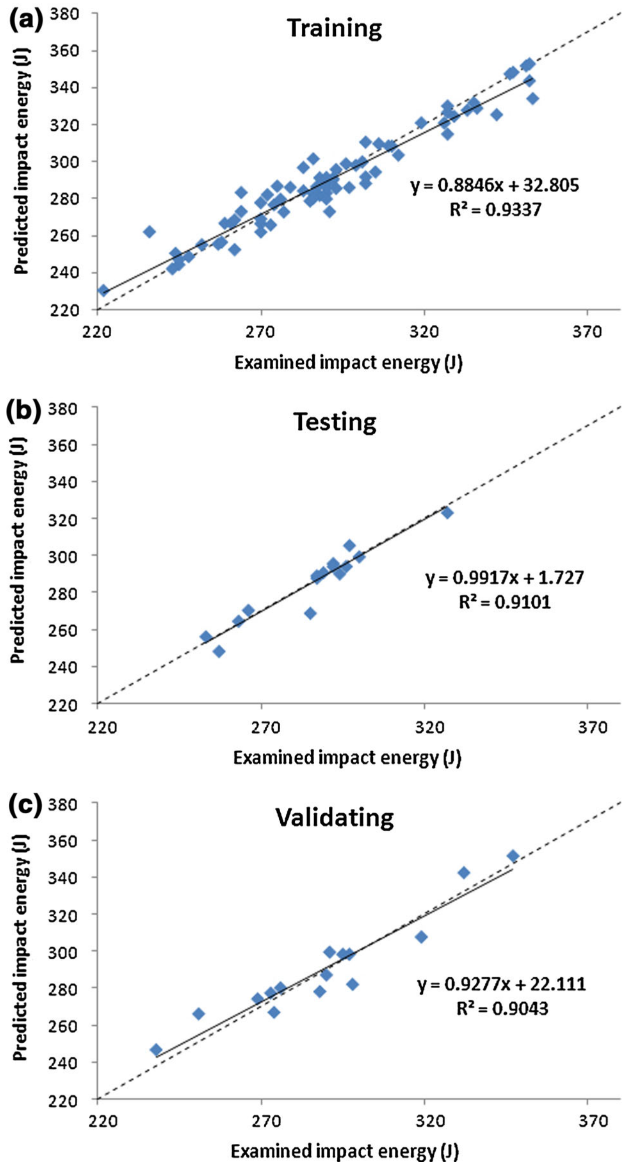

Fig. 6 The correlation of examined and predicted impact energy/toughness values in **a** training, **b** testing, and **c** validating datasets through ANN-based model

Table 2 Calculated MRE values for training, testing and validating datasets for ANN-based modelings

MRE	Training	Testing	Validating
Hardness	0.80407	1.03093	1.02505
Impact	2.13733	1.47412	2.33369

overall data can adequately predict the impact toughness and hardness of API X70 steels with an acceptable precision. In other words, there is a good agreement between the examined (experimental) toughness and hardness with the results acquired from the presented models.

4 Conclusions

In the present study, neural networks with feed forward topology and back propagation algorithms are utilized to predict impact toughness and hardness of microalloyed API X70 line pipe steels. The chemical compositions and the tensile test parameters are considered as inputs of the networks. Implemented data are selected from a wide range database containing examined results for line pipe steel plates through the pilot mill. The definition of carbon equivalent, based on the International Institute of Welding and Ito-Bessyo equations is a novel feature of the present work that enhances the applicability of the developed ANN modeling. A good approximation performance with R^2 value of 0.86 and mean relative error of 2.11 % for the overall data is obtained. It is concluded that there is a good agreement between the experimental and the predicted impact toughness and hardness values. By comparing the predicted results with the measured ones, a maximum absolute relative error of 1.1 % is obtained. The overall results show that the developed model can be artificially used (as a parallel computing system) to study the effects of all input variables on the outputs.

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