Mechanical Property Prediction of Commercially Pure Titanium Welds with Artificial Neural Network

Yanhong WEI[1)†], *H.K.D.H.Bhadeshia*[2)] *and T.Sourmail*[2)]
1) State Key Laboratory of Advanced Welding Production Technology, Harbin Institute of Technology, Harbin 150001, China
2) Department of Materials Science and Metallurgy, University of Cambridge, Cambridge CB2 3QZ, UK
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Factors that affect weld mechanical properties of commercially pure titanium have been investigated using artificial neural networks. Input data were obtained from mechanical testing of single-pass, autogenous welds, and neural network models were used to predict the ultimate tensile strength, yield strength, elongation, reduction of area, Vickers hardness and Rockwell B hardness. The results show that both oxygen and nitrogen have the most significant effects on the strength while hydrogen has the least effect over the range investigated. Predictions of the mechanical properties are shown and agree well with those obtained using the 'oxygen equivalent' (OE) equations.

KEY WORDS: Commercially pure titanium; Artificial neural networks; Mechanical properties; Weld

1. Introduction

Commercially pure (CP) titanium is strengthened by the interstitial elements, *i.e.* oxygen, nitrogen and carbon as well as by substitutional elements such as iron. Therefore, those elements should have some effects on the mechanical properties of weld metal of CP titanium. Because the cooling rate controls the grain size of the weld metal, it is expected to have an influence on its mechanical properties. Effects of those variables on mechanical properties of CP titanium welds have been ongoing for many years[1~9]. In particular, the so-called 'oxygen equivalent' (OE) empirical equations have been formulated which relate the effects of composition and welding parameters to mechanical properties of the welds of CP titanium[10,11].

Equation (1) is an improved oxygen equation and its relationships with the mechanical properties of CP titanium welds are followed by Eq.(2~7)[11,12].

$$\mathrm{OE} = 2\mathrm{C} + 3.5\mathrm{N} + \mathrm{O} - 0.14\mathrm{Fe} \quad (1)$$

$$\text{While, } \mathrm{UTS} = -130.64\mathrm{OE}^2 + 167.01\mathrm{OE} + 39.042 \quad (2)$$

$$\mathrm{YS} = -76.709\mathrm{OE}^2 + 133.08\mathrm{OE} + 31.843 \quad (3)$$

$$\%\mathrm{Elongation} = 292.72\mathrm{OE}^2 - 242.84\mathrm{OE} + 64.036 \quad (4)$$

$$\%\mathrm{ROA} = 225.2\mathrm{OE}^2 - 244.12\mathrm{OE} + 81.406 \quad (5)$$

$$\mathrm{VHN} = -925.04\mathrm{OE}^2 + 835.11\mathrm{OE} + 47.659 \quad (6)$$

$$\text{Rockwell B} = -171.44\mathrm{OE}^2 - 242.84\mathrm{OE} + 64.036 \quad (7)$$

where, UTS–ultimate tensile strength, YS–yield strength, ROA–reduction of area, VHN–Vickers hardness, Rockwell B–Rockwell B hardness.

According to the investigators, the effect of cooling rate on OE is small and can probably be ignored for most of single pass applications of gas tungsten arc welding processes, and the effect of hydrogen on OE equation is also small and probably can be ignored based on prior art and its low concentration on CP grade 2 titanium.

† Prof., Ph.D., to whom correspondence should be addressed, E-mail: yhwei@hit.edu.cn.

To farther understand the effects of elements and cooling rate on mechanical properties of CP titanium welds, artificial neural network (ANN) was used to develop models with similar data input of OE equations . A neural network is a general method of regression analysis in which a very flexible non-linear function is used to fit the experimental data. The details of this method have been extensively reviewed[12,13] and are therefore omitted in this paper. The method has also been proved very useful and effective for mechanical properties modelling of welds or parent materials[14~17]. However, most of these models are for steels and few for titanium welds. The present work therefore aims at developing artificial neural network models for CP titanium weld strength with a commercial neural network software[18].

2. Model Description

2.1 Input/output

As CP titanium is strengthened by the interstitial elements, *i.e.* oxygen, nitrogen and carbon as well as by the substitutional element iron, these elements should be taken into consideration. For welding joints, cooling rate is known to affect the cast grain size of weld metal and has an effect on weld properties. As a result, the general scheme of the models is described in Fig.1.

As shown in Fig.1, the input parameters for ANN models are chemical compositions and welding cooling rate. The output of the models is one of mechanical properties namely UTS, yield strength, elongation, ROA, Vickers hardness and Rockwell B hardness. At present, there are 39 data records for models of UTS, yield strength, elongation and ROA, and 45 data records for Vickers Hardness model and 63 data records for Rockwell B Hardness model.

2.2 Neural network training

Training is a process to fit the experimental data in the databases with the neural network. Half of the data are used for training and half of the data pairs are used to test the models. The features of those models are demonstrated in test error, perceived level of noise, log

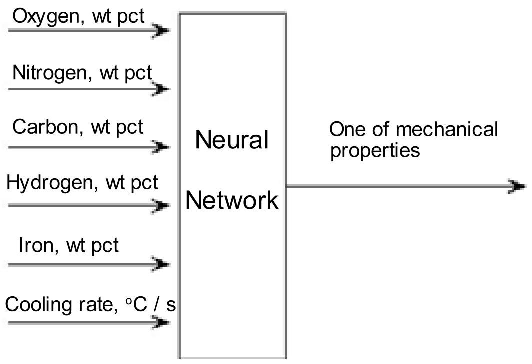

Fig.1 Schematic model of artificial neural network for modeling mechanical properties of CP titanium welded joints

predictive error (LPE), and combined error of committee.

The test error and perceived level noise are used to evaluate the performance of a single model as shown in Fig.2 which indicates that the test error and perceived level of noise tend to be smaller with more hidden units. The LPE is used to evaluate the performance of different models (Fig.3). The bigger the LPE, the better the model. The detail of LPE is explained elsewhere[12,13]. As the complexity of a model depends on its number of hidden units, models with different numbers of hidden units will give different predictions. For this reason, the training process involves the training of a large number of models with different numbers of hidden units (20 models in the context). Those models then ranked according to how they perform on unseen data. Most of the time, a combination of the best models (committee) perform better than a single model. To determine the optimum number of models to use in a committee, the combined prediction error is calculated for an increasingly large number of models. Most of the time, this combined error presents a minimum which corresponds to the optimum number of models to be used as shown in Fig.3(b).

3. Results and Discussion

3.1 Comparison of ANN models with OE equations

OE equations have been used to predict the mechanical properties of CP titanium welds[10,11]. To verify the ANN models in the context, comparisons were made between ANN models and OE equations on the same condition in Fig.4.

According to Fig.4, predictions with ANN models and OE equations are in good agreement with experimental results, and some ANN models such as Elongation, ROA and VHN models improve appreciably compared with OE

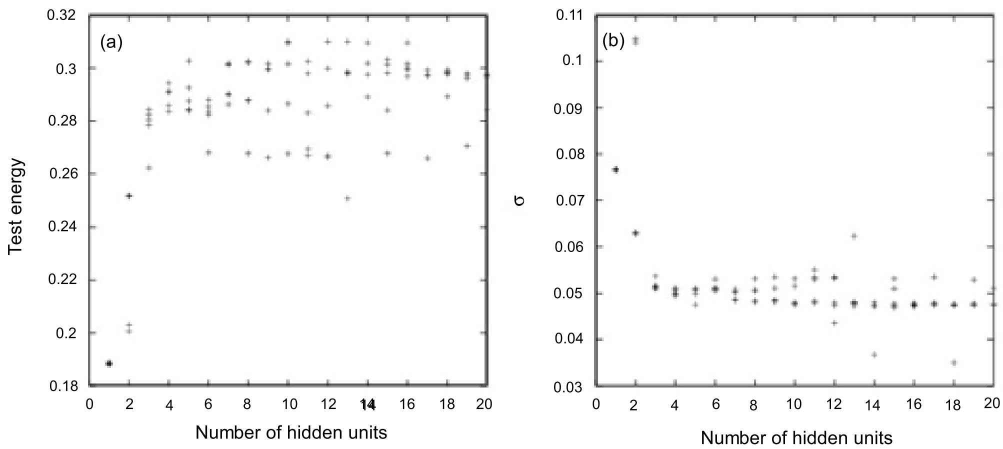

Fig.2 Test error (a) and perceived level of noise (b) of yield strength model

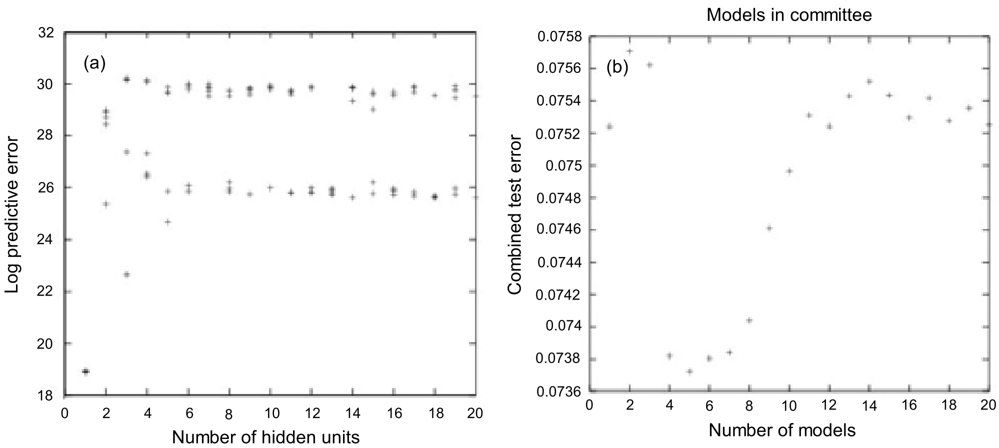

Fig.3 Log predictive error (a) and combined test error (b) of the Vickers hardness model

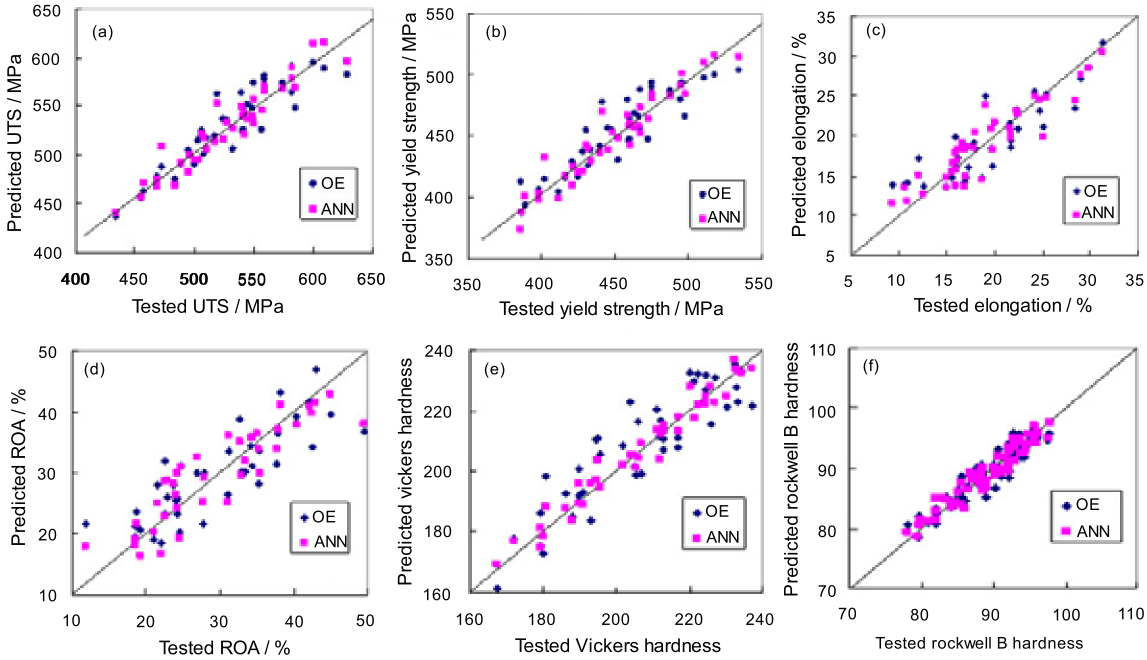

Fig.4 Comparison of predictions between ANN models and OE equations (a) UTS, (b) yield strength, (c) elongation, (d) ROA, (e) vickers hardness and (f) rockwell B hardness

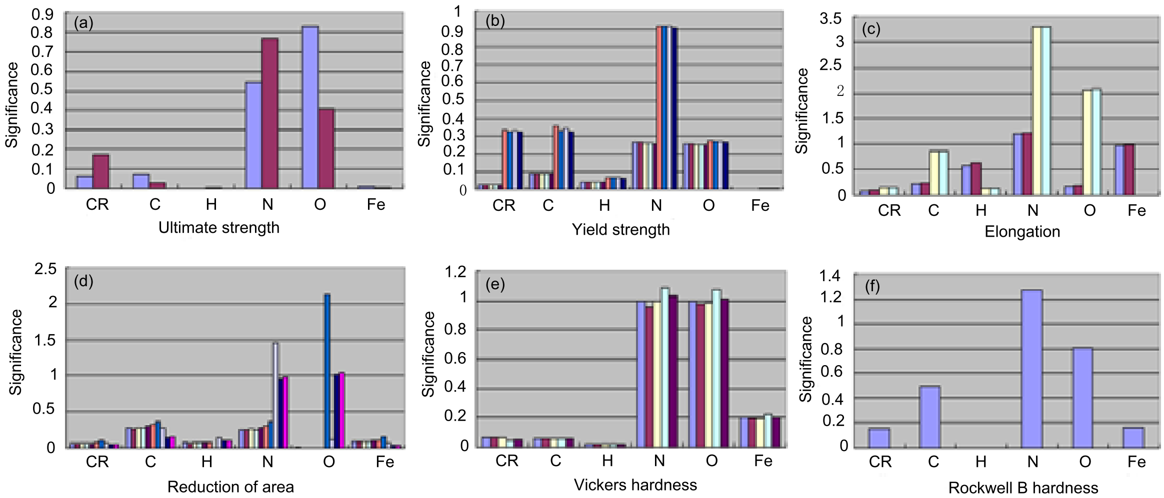

Fig.5 Significances of variables in different models (a) UTS models, (b) yield strength models (c) elongation models, (d) ROA models, (e) vickers hardness models, and (f) rockwell B hardness model

equations. As a result, ANN models can be used to predict mechanical properties of CP titanium welds.

3.2 Significances of the variables in different ANN models

Based on ANN models the significances of different variables of the models are obtained as shown in Fig.5.

In UTS models, two best models are combined to make the model committee to predict the UTS. The significances from the biggest to the smallest are oxygen, nitrogen, cooling rate, carbon, iron and hydrogen.

For yield strength model, the model committee consists of four models and the significances of the variables are in the following declining sequences: nitrogen, carbon, cooling rate, oxygen, hydrogen and iron, but the significances of carbon, cooling rate and oxygen are only slightly different.

Four models form the model committee for predicting elongation and significances of variables from the biggest to the smallest are in the following order: nitrogen, oxygen, iron, hydrogen and cooling rate.

In the Vickers hardness model, the significances of variables are in following sequences: nitrogen, oxygen, iron, cooling rate, carbon and hydrogen. The nitrogen is the most significant variable.

There are ten models in the ROA combined model committee. The most important variables are oxygen, then nitrogen. Other variables are less important.

For the Rockwell B hardness model, nitrogen is the most significant variable. Following nitrogen are oxygen, carbon, iron, cooling rate and hydrogen. Six models are combined to form the model committee.

It can be therefore concluded that, nitrogen and oxygen have the greatest influences while hydrogen has the

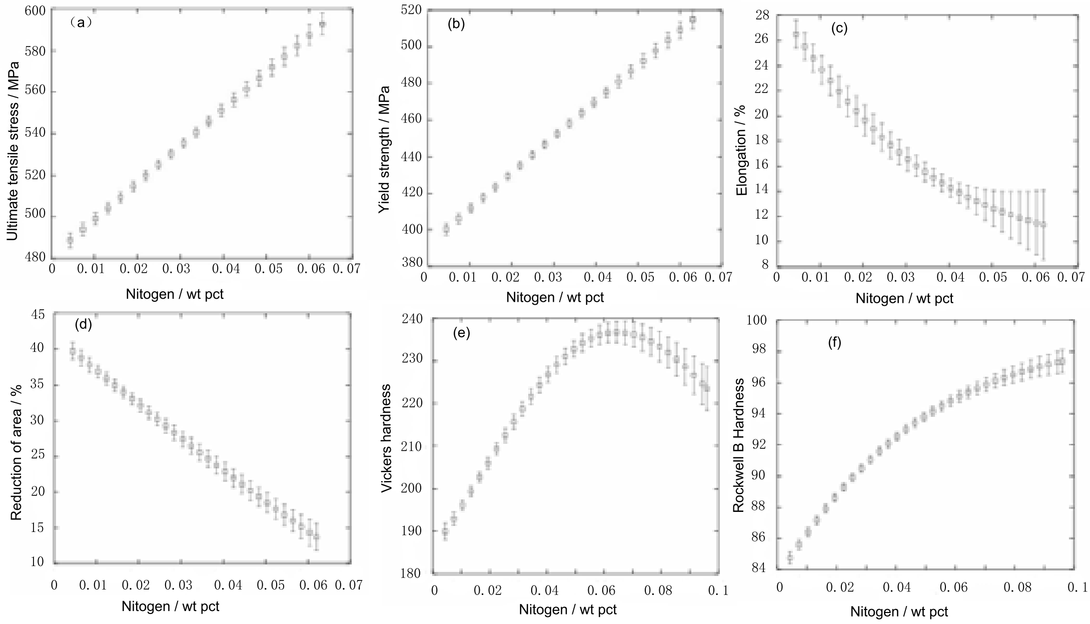

Fig.6 Predictions of mechanical properties content nitrogen ANN models (a) UTS, (b) yield strength, (c) elongation, (d) ROA, (e) vickers hardness, and (f) rockwell B hardness

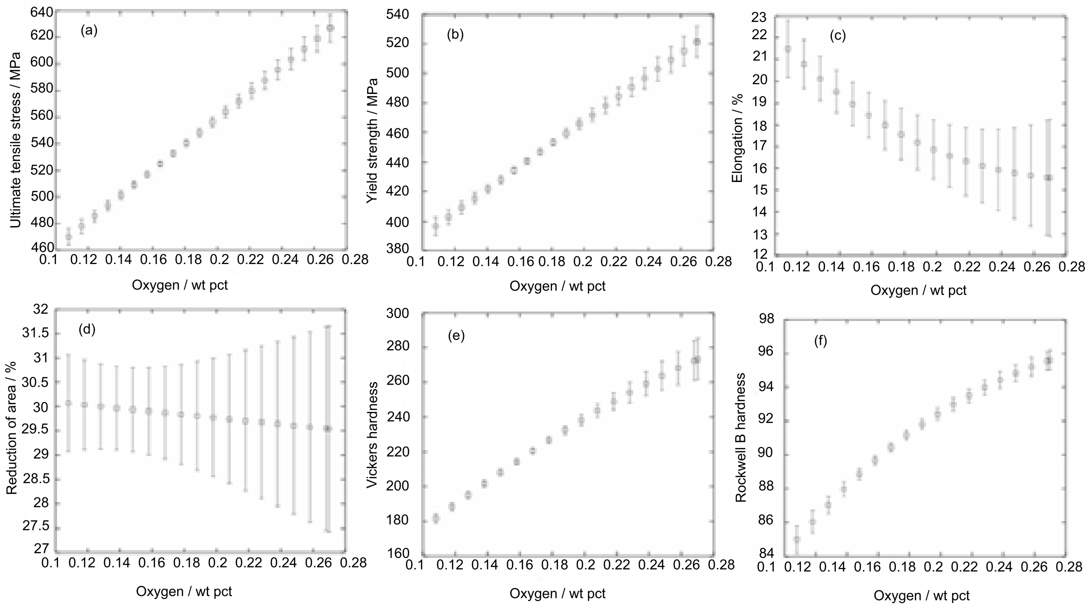

Fig.7 Predictions with oxygen content based on ANN models (a) UTS, (b) yield strength, (c) elongation, (d) ROA, (e) Vickers hardness, and (f) Rockwell B hardness

least influences on strength of CP titanium welds, which accord well with previous research works[10,11]. It was pointed out that the cooling rate had little effect on mechanical properties and was therefore omitted in the OE equations in previous study[10,11], but it is found here that for UTS model its influence is greater than that of carbon and iron as shown in Fig.5(a) and for yield strength model its influence is greater than that of oxygen and iron, and nearly equals to that of carbon as shown in Fig.5(b).

3.3 Influence of variables on mechanical properties based on ANN models

3.3.1 Nitrogen Predictions were made with different nitrogen based on ANN models as shown in Fig.6. As mentioned above, nitrogen is an important interstitial element which has significant effect on strength. As shown in Fig.6, with increasing nitrogen the UTS, yield strength, and Rockwell B hardness increase greatly, and elongation and ROA decrease obviously, which accord well with the common understanding of the effect of nitrogen on mechanical properties of CP titanium welds. For Vickers hardness, before nitrogen reaches 0.063 wt pct, it increases, and after that it decreases.

3.3.2 Oxygen Oxygen is another significant element that controls the mechanical properties of CP titanium so that CP titanium is classified by the content of oxygen and iron. As the content of these elements increases, strength increases but elongation decreases[19]. The influences of oxygen content on CP titanium welds are shown

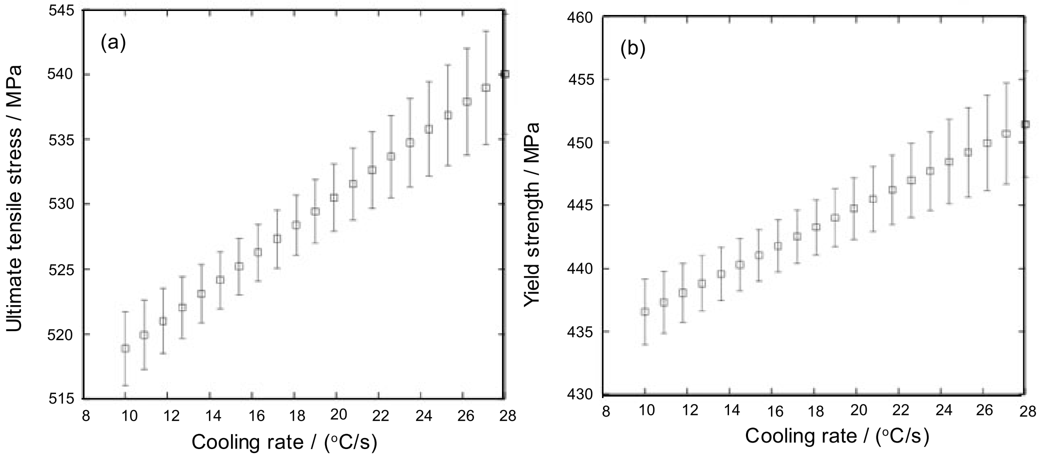

Fig.8 Prediction with cooling rate based on the ANN model UTS (a), yield strength (b)

in Fig.7.

3.3.3 Cooling rate As mentioned above, cooling rate controls the grain size of the weld metal so it has influence on the mechanical properties of weld metal too. From the significances of cooling rate shown in Fig.5, it is the third important variable in both UTS model and yield strength model while for other four models it is nearly the least significant variable next to hydrogen. Therefore, only the influences of cooling rate on UTS and yield strength are shown in Fig.8. As can be seen, with increasing cooling rate, UTS and yield strength increase appreciably, which confirms that it has effect although it is not big.

4. Conclusion

The ANN models are developed for mechanical properties modeling of CP titanium welds including UTS, yield strength, elongation, ROA, Vickers hardness and the Rockwell B hardness. The models accord well with the OE equations used to predict the mechanical properties of CP titanium welds. The effects of elements and cooling rate on mechanical properties of CP titanium welds are shown clearly, which provides a deep understanding of relationship among the factors that control strength of CP titanium welds. It is confirmed that nitrogen and oxygen are the most significant variables for mechanical properties, and the hydrogen has the least influence while the cooling rate is more important than carbon and iron with the UTS model, and more important than oxygen and iron, and equally important with carbon in the yield strength model.

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