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Practical Model for Predicting Beta Transus Temperature of Titanium Alloys

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Abstract The β-transus temperature in titanium alloys plays an important role in the design of thermo-mechanical treatments. It primarily depends on the chemical composition of the alloy and the relationship between them is non-linear and complex. Considering these relationships is difficult using mathematical equations. A feed-forward neural-network model with a back-propagation algorithm was developed to simulate the relationship between the β-transus temperature of titanium alloys, and the alloying elements. The input parameters to the model consisted of the nine alloying elements (i.e., Al, Cr, Fe, Mo, Sn, Si, V, Zr, and O), whereas the model output is the β-transus temperature. The model developed was then used to predict the β-transus temperature for different elemental combinations. Sensitivity analysis was performed on a trained neural-network model to study the effect of alloying elements on the β-transus temperature, keeping other elements constant. Very good performance of the model was achieved with previously unseen experimental data. Some explanation of the predicted results from the metallurgical point of view is given. The graphical-user-interface developed for the model should be very useful to researchers and in industry for designing the thermo-mechanical treatment of titanium alloys.

Key words titanium alloys, β transus temperature, neural networks, sensitivity analysis.

1. Introduction

Increased use of titanium alloys is occurring due to their lower modulus, superior biocompatibility, and strength to weight ratio and enhanced corrosion resistance. The major phases present in titanium alloys are alpha(hcp) and beta (bcc). The final microstructure and mechanical properties depend heavily on the thermo mechanical processing (TMP) route. The β-transus temperature(at which alpha + beta phase converts to beta phase) plays a key characteristic role in TMP. A wide variety of microstructure can be obtained depending on the materials is processed above or below β-transus temperature. Beta transus temperature is the basic reference point to design a treatment. Hence the estimation of beta transus temperature is very important and crucial. Determination of β-transus temperature is time consuming, expensive and laborious. β-transus temperature is sensitive to alloy composition and estimation of the relationship between β-transus temperature and alloying elements is vital. There are number of regression models are developed to relate between the composition and β-transus temperature and their predictions are limited use and the results differing with others.[1-4] Biologically inspired artificial neural networks (ANN's) modeling tools is an alternative and the application of ANN's in materials science field grown exponentially.[5-7] The advantage of ANNs is that relationship need not be specified in advance and do not require any assumptions since the method itself establishes relationship through training process. They are particularly valuable where inputs are related or missing or the systems are nonlinear. Guo *et al*. used neural networks model to predict β-transus temperature by using commercial MATLAB software.[8] Those predictions are few deviations from experimental values and they claimed, it is due to insufficient data. First author predicted beta transus temperature by extrapolation of beta phase volume fraction as a function of Al, V, Fe, O, N and heat treatment temperature. Hence our main objective is to build a practical, reliable, and effective model to minimize the experiments required to determine β-transus temperature.

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2. Materials and Methods

2.1 Materials

Modeling system for the beta transus temperature of titanium alloys has been developed by correlating nine alloying elements Al, Cr, Fe, Mo, Sn, Si, V, Zr, and O. The database for beta transus was compiled of alpha, alpha + beta, beta titanium alloys[9-12] and Prof. W. Sha shared the compiled database.[8] The statistics of the data was shown in Table 1. A total of 201 data sets were used for developing the model and the ranges of the alloys were vast.

2.2 Brief explanation about neural networks model

In the present work, feed forward neural networks (FFNN) with back propagation algorithm(BPA) was employed and the details were summarized elsewhere.[13,14] The model was implemented using the programming languages C and Java. Fig. 1 shows the schematic diagram of the present problem. It consists of nine nodes representing composition at input layer and one node at output layer. In between these two layers are the hidden layers with number of nodes. The actual number of hidden layers and hidden nodes depends on the system and acceptable level of the model. Hidden layers are necessary to map nonlinear relationship in the system. The BPA allows to learning input - output mapping from the training samples. The training process is accomplished in two passes(forward and backward) through the network. In the forward pass, an input pattern is fed, and the outputs of all neurons in each layer are computed by choosing the initial weights(randomly generated small values in between –0.5 to +0.5). The error in the output layer is found by comparing the output with the target value. In the backward pass the weights are suitably updated so to minimize the overall training error. In doing so, two parameters, called learning rate and momentum factor are introduced for controlling the size of the weights adjustment along the descent direction. These two parameter values(in between 0.1 to 0.9) are empirically chosen. For all patterns, *p*, the global error function, Mean sum Squared Error(MSE) is given by:

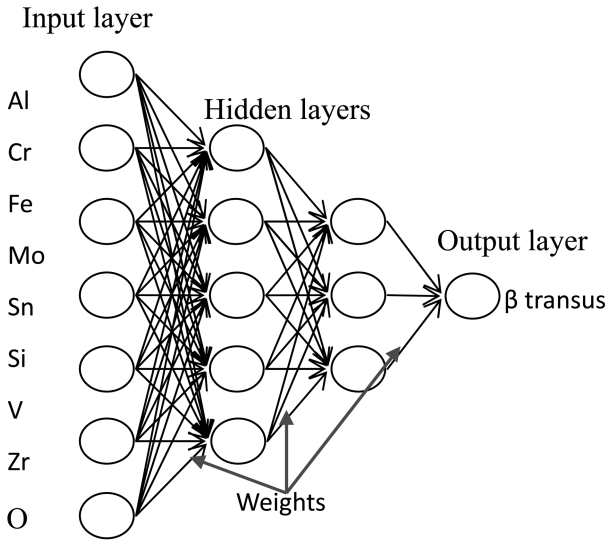

Fig. 1. Schematic diagram representing neural networks model.

$$MSE = \frac{1}{p}\sum_{p}\sum_{i}(T_{ip} - O_{ip})^2$$

where, T_{ip} is the target output and O_{ip} is the calculated output for the i^{th} input neuron for the p^{th} pattern respectively. The error function is minimized as follows:

1st Step: All weights initialized to small random values, which also incorporate bias term.

2nd Step: The network is provided with input and the desired output pairs from the training sets, learning rate, momentum term, hidden layers and number of hidden nodes in hidden layers

3rd Step: Output is calculated using sigmoid threshold function. The differences between calculated and experimental outputs were measured.

Table 1. Statistical analysis of the input and output variables(concentration in wt%) used for model development.

Variable	Number of alloys containing this element	Min	Max	Average	Standard deviation
Al	135	0	9.6	3.22	2.64
Cr	48	0	11.2	0.92	2.1
Fe	109	0	5	0.29	0.67
Mo	100	0	16.08	2.66	4
Sn	42	0	11	0.66	1.59
Si	34	0	0.5	0.03	0.09
V	64	0	20.16	2.51	4.59
Zr	41	0	11	0.12	0.13
O	152	0	0.9	0.12	0.13
β-transus(°C)	201	670	1080	892.2	100.4

4th Step: Weights are adjusted by using a BPA that starts from the output layer back to the input layer. The overall procedure is repeated iteratively commencing from 2nd step till the error reached to the desired minimum.

2.3 Performing sensitivity analysis on trained neural networks model

The optimal parameters required for the model are determined based on MSE and the average error in output prediction of the trained data.[15,16] Average error in output prediction will helps to avoid over fitting. Mean square error of 0.00001 and average error of 2.24 was achieved after 118662 iterations with two hidden layers consist of 12 hidden nodes in each layer with the learning rate of 0.4 and momentum term of 0.9. The model with this architecture is used for prediction and analysis of beta transus temperature. Many alloy developments were based on alloying elements relations and interactions. The model can be used to calculate the beta transus temperature by performing sensitivity analysis at various chemical compositions. Introduction to sensitivity analysis and performing the sensitivity analysis on trained neural network model was well recorded and reported in earlier publications.[15-22] In the present work the sensitivity analysis calculated in two ways: varying one input parameter and varying two input parameters while keeping other elements constant(zero) and studying their influences on output. The instantaneous sensitivity, S_{jk}^{P}, of kth output with respect to jth input, can be evaluated at each operating point P, as follows:

$$S_{jk}^{P} = \frac{\Delta o_k^P}{\Delta u_j^P}$$

where,

$\Delta o_K = f(u_j + \Delta u_j) - f(u_j)$

$f(\ )$ being realized in the model,

u_j^P = Nominal value of jth input variable at operating point P,

o_k^P = Corresponding nominal value of kth output variable at operating point P,

Δu_j = Very small increment in the nominal value of jth input variable.

3. Results

The performance of the model was evaluated by predicting beta transus temperature from 57 new unseen experimental data from our previous work[16] and other sources.[23,24] The comparison between the predicted and experimental beta transus temperature and the respective percentage errors were shown in Table 2.

Estimation of phase diagram of binary Ti-X(X = Al, V, Mo and O) and Ti-Al-V-Cr systems: The complete predictions of the model are voluminous, hence representative predictions were shown. The neural networks models are based on data and equations. Hence, the reason behind the predictions will be tried to explain. Fig. 2 represents the screen shots of graphical user interface designed for beta transus temperature. Binary phase Ti-Al, Ti-V, Ti-Mo and Ti-O were calculated by performing sensitivity analysis on trained model and compared with the experimental. Fig. 4 shows hypothetical multiphase titanium alloy, Ti-Al-V-Cr systems predicted by model. The beta transus temperature varied as a function of aluminum and vanadium content at different chromium additions and fixing other alloying elements to zero.

4. Discussions

The % error in prediction is less than 4.5 % for 47 data sets and in the case of 10 data sets, the error range is higher as shown in Table 2. In the case of 28 data sets belongs to alpha + beta alloys the predictions are precise and the error is less than 2 %. The higher prediction error occurred in the multi element system and especially in the case of 9 metastable beta phase alloys[24](Sample No's 49-57). By observing carefully, the reason for higher error is due to lack of sufficient beta phase alloys data and the available data is sparse.

The percentage error in prediction of the samples 7, 8, 9 and 10 are 3.9, 2.6, 0.3 and 1.4 respectively. The beta transus temperature experiments of these samples were carried out at POSCO, Pohang, Korea to evaluate the extrapolated prediction of beta phase volume.[16] Determination of β transus temperature by phase disappearing method is time consuming, expensive and difficult one. The present model can help to identify the β transus temperature with minimum error. At present we are collecting more versatile data to improve the effectiveness of the model and to make it as a generalized standard model for estimating β transus. The graphical user interface of the beta transus model is easy to use and the screen shots were shown. Fig. 2(a) shows the prediction at new instances and 2(b) shows the estimated beta transus as a function of Al and V at 5 % chromium keeping other elements to zero. A few Korean researchers in academia and industry are using the present model to estimate the β transus temperature.

The usefulness of the developed model does not end with the predictions of the beta transus, but it can be used for the examination of the data and to construct phase diagrams. For instance, it is useful to predict the effect of a single element or two on the beta transus temperature keeping all the remaining elements unchanged by sensitivity analysis.[15,16]

Beta transus temperature for pure titanium is around

Table 2. Prediction of beta transus temperature for unseen α, α+β and β titanium alloys.

S.No	Al	Cr	Fe	Mo	Sn	Si	V	Zr	O	Nature of alloy	A	P	(% E)	Ref.
1			0.2						0.18	α	890	884.4	−0.6	24
2			0.3						0.25	α	915	903.4	−1.3	24
3			0.3						0.35	α	920	928.0	0.9	24
4			0.5						0.4	α	950	941.6	−0.9	24
5	5				2.5					α	1040	1018.3	−2.1	24
6				0.3						α	880	878.9	−0.1	24
7	7		0.01				1.5		0.15	α	1066	1024.0	−3.9	16
8	6.85		0.13				1.6		0.17	Near α	1044	1017.0	−2.6	16
9	6.19		0.19				4.05		0.12	α + β	989	992.3	0.3	16
10	6.33		0.19				4		0.17	α + β	998	983.8	−1.4	16
11	4.85		0.1				4.5		0.2	α + β	960	959.5	−0.1	23
12	4.76		0.4				4.3		0.1	α + β	925	946.6	2.3	23
13	6.55		0.4				4.4		0.1	α + β	1000	992.5	−0.7	23
14	6.55		0.4				4.4		0.1	α + β	975	1002.8	2.8	23
15	5.64		0.3				3.8		0.1	α + β	970	979.9	1.0	23
16	4.766		0.1				3.3		0.1	α + β	947	969.8	2.4	23
17	6.514		0.1				4.3		0.1	α + β	969	1002.4	3.4	23
18	6.495		0.1				3.3		0.2	α + β	1012	995.1	−1.7	23
19	4.79		0.4				3.4		0.2	α + β	963	955.2	−0.8	23
20	4.85		0.11				4.45		0.198	α + β	960	959.4	−0.1	23
21	4.76		0.39				4.27		0.072	α + β	925	948.2	2.5	23
22	6.55		0.407				4.38		0.197	α + β	1000	976.9	−2.3	23
23	6.55		0.394				3.38		0.071	α + β	975	1007.3	3.3	23
24	5.64		0.252				3.83		0.135	α + β	970	977.6	0.8	23
25	4.766		0.11				3.297		0.08	α + β	947	970.7	2.5	23
26	6.514		0.11				4.29		0.079	α + β	969	1004.9	3.7	23
27	6.495		0.107				3.313		0.19	α + β	1012	996.5	−1.6	23
28	4.79		0.39				3.35		0.196	α + β	963	955.9	−0.7	23
29	8			1			1			α + β	1040	1046.9	0.7	24
30	6			1	2	0.1		1.5		α + β	1015	993.9	−2.1	24
31	5.9			0.4	2.6	0.45		3.8		α + β	1010	1048.3	3.8	24
32	2.5			1	11	0.2		5		α + β	945	985.2	4.3	24
33	6			0.5		0.25		5		α + β	1020	1011.6	−0.8	24
34	5.5			0.25	3.5	0.3		3		α + β	1015	1030.8	1.6	24
35	5.8			0.5	4	0.35		3.5		α + β	1045	1033.7	−1.1	24
36	5			0.8	6	0.25		2		α + β	1005	1048.0	4.3	24
37	6			2	2	0.1		4		α + β	995	1002.8	0.8	24
38	5			2	5	0.25		2		α + β	980	1024.0	4.5	24
39	3						2.5			α + β	935	939.9	0.5	24
40	6						4			α + β	995	1006.2	1.1	24
41	6				2		6			α + β	945	977.3	3.4	24
42	4			4	2	0.5				α + β	975	1050.7	7.8	24
43	5			4	2	0.25		2		α + β	960	961.0	0.1	24
44	6	2		2	2	0.25		2		α + β	970	975.6	0.6	24
45	6			6	2			4		α + β	940	1087.2	15.7	24
46	6		2			0.1				α + β	1015	941.2	−7.3	24
47	4.5	1.5		5						α + β	935	961.9	2.9	24
48	5	4		4	2			2		α + β	890	1041.6	17.0	24
49	3	11					13			β	720	736.6	2.3	24
50				11.5	4.5			6		β	760	857.2	12.8	24
51	3	6		4			8	4		β	795	659.9	17.0	24
52	3		2				10			β	800	772.7	−3.4	24
53	3	3			3		15			β	760	699.3	−8.0	24
54	3			15		0.2				β	815	763.9	−6.3	24
55	1.5		4.5	6.8						β	810	708.0	12.6	24
56	5	2	1	4	2			4		β	890	955.3	7.3	24
57	4.5		2	2			3			β	900	891.7	−0.9	24

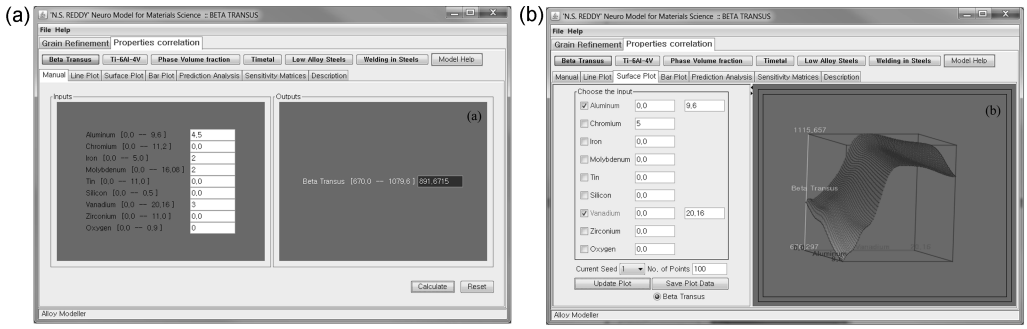

Fig. 2. Screen shots of the user interface of the model (a) prediction of beta transus temperature Ti-4.5Al-2Fe-2Mo-3V alloy(Sample no 57 in Table 2) (b). Surface plot of the beta transus as a function of Aluminum and Vanadium at 5 % Chromium.

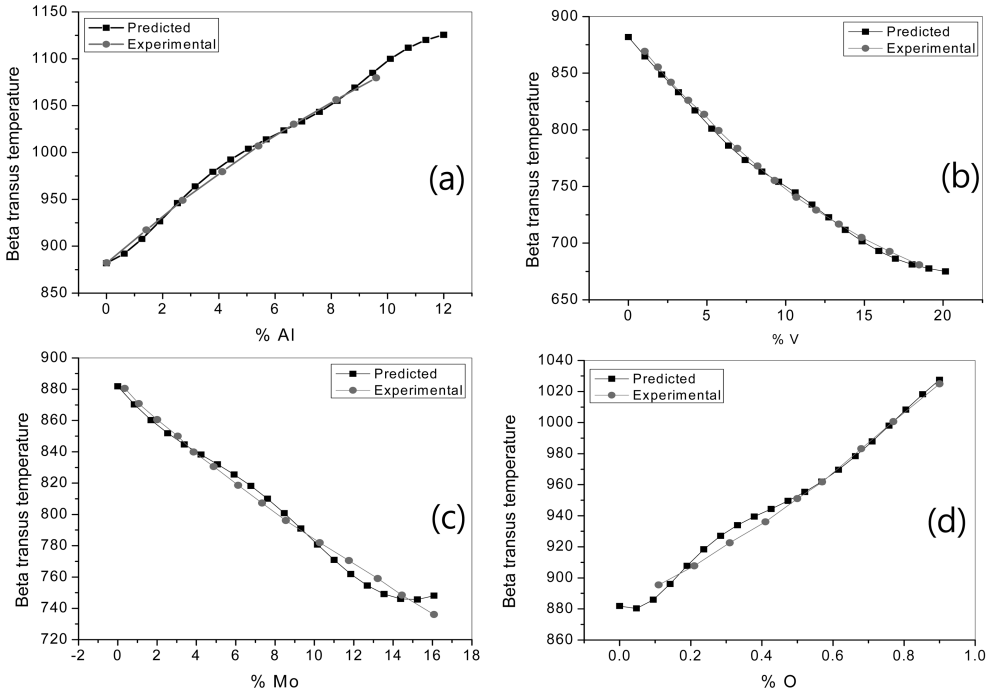

Fig. 3. Predicted and experimental beta transus temperature of (a) Ti-xAl alloy, (b) Ti-xV alloy, (c) Ti-xMo alloy, (d) Ti-xO alloy.

882 °C. In general, the amount of Al in titanium alloys is usually limited to 7.0 %, and the available data for higher % Al is sparse. However, to test model predictability, we asked the model to predict the β transus temperature up to 12 % Al addition keeping other elements as zero. As Al increases from 0 % to 12 %, the beta transus temperature increased from 882 °C to 1125 °C shown in Fig. 3(a). Even though, the maximum experimental data available for limited to 9.6 %, the predictions beyond the experimental data are reasonable and quite acceptable. The model predictions with increase in vanadium from 0 to 20 % resulted the beta transus is dropped from 882 °C to 675 °C represented in Fig. 3(b). The increase in molybdenum from 0 to 16 % caused the decrease in beta transus temperature to 730 °C shown in Fig. 3(c). The increase in oxygen from 0 to 1 % raised the beta transus temperature to 1029 °C and shown in Fig. 3(d).

Al and O are alpha stabilizers and increase the beta transus temperature. V and Mo are beta stabilizers and reduce the beta transus temperature. This is well established phenomenon and the model predictions are in good agreement with it and error in comparison with the experimental data is minimal. Most importantly, Guo *et al.*[8] used same data and predicted the binary Ti-X(X = Al, V, Mo, O) systems and the present model outperformed their model predictions. As good predictions are achieved with binary phase diagrams, we tried to explore the sensitivity analysis further for multicomponent phase diagram which were not reported earlier as per authors best of knowledge.

Fig. 4. shows the estimated beta transus temperature by varying Al and V from minimum to maximum at various

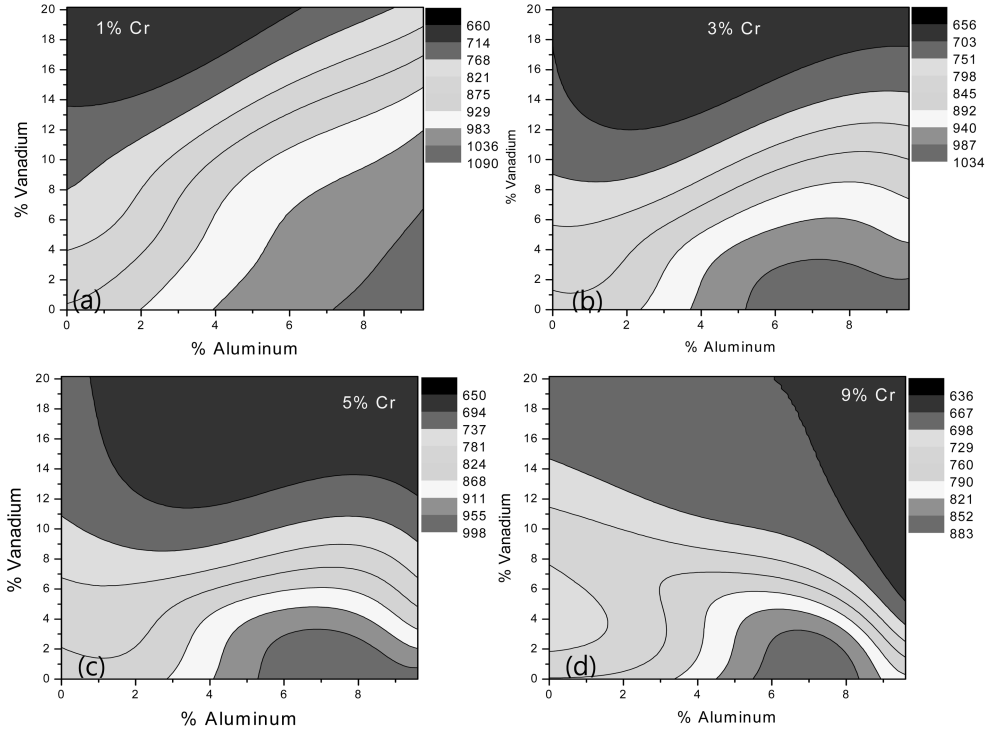

Fig. 4. Contour plot of predicted beta transus temperature of Ti-xAl-yV alloy with (a) 1 % Cr, (b) 3 % Cr, (c) 5 % Cr, (d) 9 % Cr.

at 1, 3, 5 and 9 % of Cr values. The other alloying elements were kept zero. Aluminum addition increases beta transus temperature. Vanadium and chromium decreases the beta transus temperature. These changes and the interactions between these elements are unknown, non-linear, and complex. Constructing these alloys in real life with these variations is expensive and time consuming. The predicted self-explanatory contour plots allow the range of conditions for the optimization of alloying elements for the desired β transus temperature by visual inspection. The various color bands indicate the range of beta transus temperature as a function of Al, V and 1, 3, 5 and 9 % addition of Cr. The range of aluminum and vanadium varies from 0 to 9.6 % and 0 to 20 %, respectively. We note that every point in the Figure specifies one multicomponent Ti-Al-V-Cr system. Increase in chromium percentage from 1 % to 9 % decreased the beta transus temperature ranges from 660-1090 °C to 636-883 °C. The contour shapes are becoming more complex with the increase in chromium. This beta transus temperature map can provide an insight into the absolute amount of chemical composition required to identify the process window for titanium alloys. The model can predict and analyze beta transus temperature for any combination of desired alloying elements. Table 1 show the wide ranges of compositions where infinite number of titanium alloys was feasible within the limit. Hence, the construction of the model with large number of reliable datasets(present 201 data sets) makes the model suitable for entire titanium alloys family.

5. Conclusions

The predictions with unseen experimental data show that the neural networks can model complicated and non-linear complex relationships between beta transus temperature and alloy composition. Sufficient reliable data is necessary for an effective and efficient prediction. The sensitivity analysis helps to construct the binary and multicomponent titanium alloy systems and to identify the effect of alloying elements. The predictions by the model provide useful information from relatively small experimental databases(201 data sets). On the shop-floor, a great deal of time, energy and materials can be saved to find the beta transus temperature of any unknown titanium alloys with whatever composition(within the range). The established relationships would be very useful to industries for designing their experiments, and eventually their alloy.

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