Modelling of Beta Transus Temperature in Titanium Alloys Using Thermodynamic Calculation and Neural Networks

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ABSTRACT

Two different methods, thermodynamic calculation and artificial neural networks modelling, have been used to model the beta transus temperature of titanium alloys. Results from either method agree with experimental results very well. The well-trained neural network model has also been successfully used to predict the beta transus temperature of new alloys which showed good performance. Influences of alloy elements Al and Mo on the beta transus temperature in Ti-Al and Ti-Mo binary system have also been modelled; the results are again in good agreement with experimental data. In addition, the appropriate concentration range of both methods for each element has been listed.

Key words: Modelling, Beta transus, Thermodynamics, Neural network

1. INTRODUCTION

Materials production technology requires a detailed knowledge of process parameters and the effects of these parameters on product properties. Essentially there are two different ways of predicting these effects. Firstly one can develop a model which describes physical relations between parameters and product properties, and verify this model using experiments. Alternatively, a model can be created by applying statistical techniques to existing production data. The advantage of the former method is that it is associated with a basic understanding of the mechanism of the phenomenon. However, an explicit physical model of the production process requires knowledge of all relations between production parameters, microstructure and final properties which are usually difficult to obtain. In this aspect, the advantage of the latter approach is that it can cope with incomplete dataset without prior knowledge of the physical background of the processes occurring. However, some background knowledge might be needed to interpret the statistical or predicted results.

In the current work, both approaches were used to model the alpha to beta transformation in titanium alloys. In recent years, phase transformation modelling of titanium alloys has become much attractive as a means toward full control of the microstructure through processing so as to more thoroughly exploit the superior combined properties of these remarkable materials. Because of the potential of strengthening by the control of microstructure, knowledge of fundamental properties such as the β-transus temperature and volume fraction of α or β as a function of temperature is a critical factor in alloy design and selection of processing parameters. Modelling of beta transus temperature is a suitable starting point as it has relatively little relation with production parameters, which makes the problem much simpler, compared with modelling of mechanical properties such as tensile strength and hardness, and corrosion resistance.

Thermodynamic theories of phase transformation in materials have been well developed and computer packages have been produced which can be used to calculate the equilibrium status at different conditions, such as MTDATA and Thermo-Calc [1]. The first method in this paper is to use the Thermo-Calc (TC) package, which was developed at the Royal Institute of Technology in Sweden, particularly for thermodynamic calculation of materials based on various databases. The database specially for calculation of titanium alloys is the Ti-Data database assembled by ThermoTech Ltd. in the United Kingdom [2].

The second method is to use artificial neural networks (ANNs) to construct a quantitative black-box model for titanium alloys, which connects input data to output data without making any prior assumptions on the type of functional dependence. Usually, the input data can be processing conditions and the output data the mechanical or physical properties of the final product. In the present study, the inputs and output are much simpler which are the chemical composition of each alloy element and the beta transus temperature of an alloy, respectively. Such method has been successfully used to model the austenite formation and mechanical properties of steels [3-7]. More information about these two methods is detailed in the following sections.

2. THERMODYNAMIC CALCULATION USING THERMO-CALC

2.1 METHOD

A traditional way of materials research is to construct a physical model based on a theoretical concept which is then verified with experimental data. Continuing improvement of the model is required to increase its level of generalisation as new phenomena are discovered. Ti-based alloys, although in wide application only since 1940's, were one of the first material types to which thermodynamic calculations such as phase diagram were applied [8,9]. Improvements in modelling and the increase in computing power have since enabled very accurate predictions to be made for phase equilibria in industrial multicomponent alloys. Saunders and Chandrasekaran showed that in a Ti-6Al-4V alloy with O, C and N included, the effect of O on the β-transus could be accurately predicted [8].

Based on various thermodynamic databanks available, Thermo-Calc has been developed which is the program used in the present work. The main method of this package is a Gibbs free energy minimisation process, and it can handle single equilibrium, property diagrams or phase diagrams with up to 20 elements. In this paper, modelling work of titanium alloys using Thermo-Calc has been carried out, using Ti-Data, a database for Ti-based alloys, which takes 15 elements (Ti-Al-Cr-Fe-Mo-Nb-Si-Sn-Ta-V-Zr-C-O-N-B) into account. Detailed information about the Thermo-Calc package and Ti-Data database can be referred to Refs. [10] and [2], respectively.

2.2 RESULTS

Thermodynamic calculation of the beta transus temperatures of 50 kinds of titanium alloys has been carried out in the present work. The chemical composition and experimental beta transus data of these alloys are obtained from references [11-15]. The maximum values for O and Fe in alloy specification were used in the calculations. The average composition was adopted for all the other elements except C and N. It was found that results without C and N were more accurate compared with results calculated with C and N being taken into account. Even if only 1/2 [maximum] of C and N were introduced into calculation it would lead to a much overestimated beta transus temperature. This is because their real contents are far below their nominal maximum amount [16]. As C and N strongly influence the beta transus temperature, it is reasonable that the beta temperature would be overestimated when their amounts are overestimated. Therefore, it is recommended that C and N had better not be taken into account at this stage no accurate data are available. As O and Fe always exist, they were given values of 0.1%wt and 0.2%wt separately when no data were available (as inpurities their concentrations are around these values). Figure 1 shows the comparison of experimental results and the predicted results. Some statistical analysis of these results is given in Table 1.

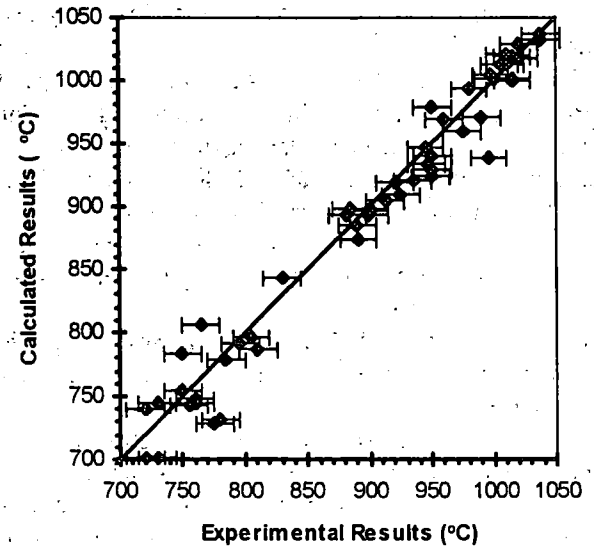

Figure 1 Comparison of experimental results and calculated results using Thermo-Calc

Table 1. Statistical analysis of experimental and Thermo-Calc results of β-transus

	Experimental results	Calculated results
Max / Min (°C)	1038 / 720	1037 / 702
Mean value (°C)	900	896
Standard deviation (°C)	101	103
Mean error (°C)	-4	
Error deviation (°C)	19	

In Table 1,

$$\text{Mean error} = \frac{1}{n}\sum_{i=1}^{n}(x_i - x_{i0}) \quad (1)$$

$$\text{Error deviation} = \sqrt{\left(n\sum(x_i - x_{i0})^2 - \left(\sum(x_i - x_{i0})^2\right)\right) \Big/ n(n-1)} \quad (2)$$

where x_i is the calculated result, x_{i0} is the experimental value and n is the number of alloys. It can be seen that thermodynamic calculation using Thermo-Calc has given reasonable results for most cases. However, for some alloys such as Ti-13V-11Cr-3Al and Ti-4Al-4Mo-4Sn-0.5Si, notable errors arose while Thermo-Calc were used to calculated their beta transus temperatures. Explanation for some cases is that, as declared by the Ti-Data database, there are some compositional limitations to be recognised while using this Ti-Data database which are stated in Appendix. Attention should be paid to when thermodynamic calculation is carried out on alloys such as Ti-13V-11Cr-3Al, whose chromium content 11%wt is far out of the limited amount 5%wt. Errors linked with alloys like Ti-4Al-4Mo-4Sn-0.5Si is due to not taking C into account during the calculation whereas it was added on purpose here with an amount of 0.05-0.20% [11]. The calculated result is 1034°C, close to its experimental datum 1050°C. The incompleteness of the Ti-Data database may also cause errors. As the influence of C and N were not taken into account, it is understandable that the average of the calculated results is slightly lower than that of the experimental results since small amount of C and N has much influence on increasing the β-transus temperature.

Nevertheless, thermodynamic calculation with Thermo-Calc package provides a way to predict the beta transus temperature of alloys. Beside this, it can also be used to calculate the phase transformation fraction, and element distribution in different phases at certain temperature [1,10]. Upgrading of the database, and taking more elements and species into account may lead to more accurate results of calculation in the future.

3. ARTIFICIAL NEURAL NETWORK MODELLING

As aforementioned, another modelling approach is to derive a mathematical model based on process data alone while ignoring the physical background of the process. A wide variety of linear statistical methods have been developed, which have proved to be powerful tools in data analysis. An artificial neural network (ANN) can also be employed, which is basically a non-linear statistical technique. ANNs are relatively easy to be employed, but, the validation of such a model is always a weak point. Usually the validation is executed statistically with separate dataset. It should be pointed out that the ANNs are not well suited for extrapolation. It can be considered as a 'black box' operation which can link input data to output data in a very clever but uncontrollable way. In extreme cases, ANNs can lead to absurd results. Therefore, background knowledge is needed to evaluate the credibility when they are used to do prediction.

For the modelling of beta transus temperature, input data is the chemical composition of each alloy. Other less important factors which might influence the beta transus temperature have not been taken into account at this stage due to lack of data. The output of the neural network is only one, the beta transus temperature. Detailed information about the working principle of ANNs can be referred to elsewhere [17,18].

3.1. MODELLING METHOD

A number of techniques of artificial neural network modelling have been developed and investigated over the years by mathematicians. The most widely studied is 'backpropagation', which is used in the current work. Backpropagation provides a way of using examples of a target function to find the coefficients that make a certain mapping function approximate the target function as close as possible. A fully connected three-layer feedforward network is employed to visualise how the computation is carried out (Figure 2).

The network consists of three layers: the input, hidden, and output layers. Each node in the input layer brings into the network the value of one independent variable. The nodes in the hidden layer do most of the work. Each of the output nodes computes one dependent variable. This network is fully connected in that there are links between all the nodes in adjacent layers. There is a separate link from each input node to each hidden node and from each hidden node to each output node. Each link has a connection strength, or weight, which is stored in and maintained by the node on the receiving end of the link. The network operates in two modes: mapping mode and learning mode. In mapping mode, information flows forward through the network, from inputs to outputs. In learning mode, the information flow alternates between forward and backward. In mapping mode, the network processes one example at a time, producing an estimate of the values of the dependent variables (weights) based on the values of the independent variables for that example. The schematic diagram of the mapping and learning is illustrated in Figure 3.

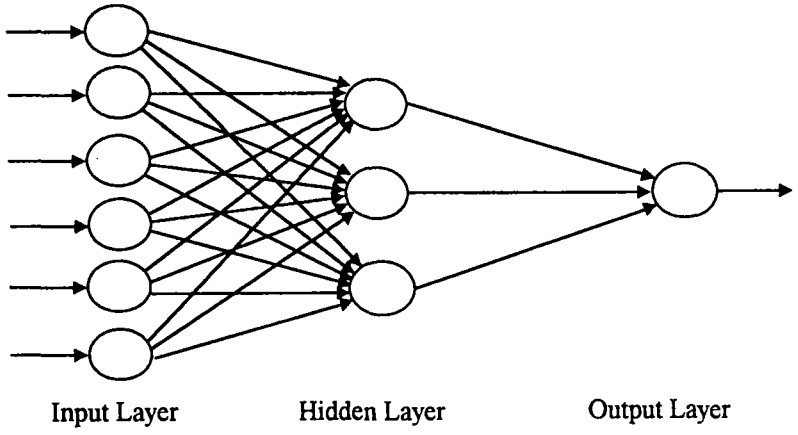

Figure 2 Structure of a neural network

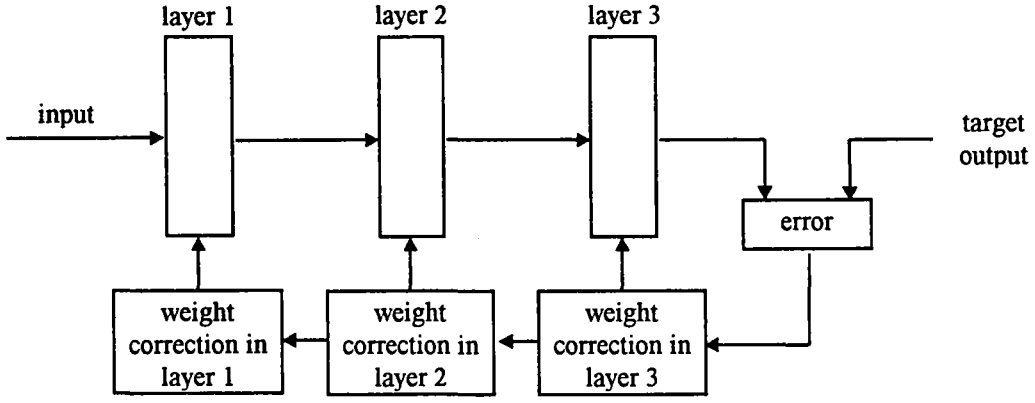

Figure 3 Schematic diagram of mapping and learning

In simplified mathematics terms, the computation can be described as follows, for a network with three layers. The numbers of nodes of input, hidden and output layers are I, J, K, respectively. The computation takes place in the following order:

(1) Given input variables x_i, where i = 1, I;

(2) $u_i = g_1(a_i x_i)$, for i = 1, I;

(3) $y_j = b_{0j} + \sum_{i=1}^{I} a_{ij} u_i$;

(4) $v_j = g_2(y_j)$, for j = 1, J;

(5) $z_k = c_{0k} + \sum_{j=1}^{J} b_{jk} v_j$, for k = 1, K, where z_k is the k-th output variable.

The above-mentioned a_i, a_{ij}, b_{jk} and c_{0k} are usually called weights; u_i and v_j are inputs to the hidden layer and the output layer, respectively; y_j is the output of the hidden layer; and g_1 and g_2 are named transfer functions. Theoretically, the transfer function can be any kind of sigmoid functions such as logistic function and hyperbolic tangent function, which are commonly used.

3.2. DATA

The dataset consisted of 9 input variables, and one output variable. The input variables are the chemical concentration of element Al, Cr, Fe, Mo, Nb, Sn, Si, V and Zr. The whole dataset includes 44 input-output data pairs. As there is only one alloy containing Ta element (1.0%wt) and one alloy containing Ni (0.8%wt), these elements were not taken into account. The output variable is the beta transus temperature. It should be noted that alloys with maximum or minimum amount of each element were put into the training instead of testing data on purpose, as neural networks cannot cope with extrapolation. Table 2 shows the dataset for modelling in a statistical term.

Table 2 Statistical analysis of the input and output variables (alloy element concentration in wt%)

Variables	Number of alloys containing this element	Min	Max	Mean	Standard Deviation
Al	39	0	7.85	3.71	2.30
Cr	8	0	11	0.64	1.93
Fe	44	0.05	5	0.65	1.05
Mo	28	0	15	2.84	4.46
Nb	5	0	7	0.28	1.11
Sn	20	0	11	1.38	2.15
Si	14	0	0.5	0.07	0.14
V	13	0	15	2.12	4.15
Zr	19	0	11	1.66	2.47
β-transus (°C)	-	700	1050	912	108

The software used in the present work is Trajan 2.1 Shareware Neural Network Simulator developed by Trajan Software Ltd., U.K. Detailed information about this package can be obtained from Ref. [19]. As the transfer function used here is logistic function

$$f(x) = 1/(1+e^{-x})$$

whose output range is (0, 1), normalisation of the output variable, the beta transus temperature, is operated by

$$x_N = (x-x_{min})/(x_{max}-x_{min})$$

where x is the beta transus of a certain alloy, x_N is the normalised value of x and x_{min} and x_{max} are the minimum and maximum values of the beta transus in the entire dataset, respectively. The same normalisation was also operated on each input variable, i.e., the concentration of each element.

3.3 RESULTS

3.3.1. Model performance

As Kurt et al. [20] have shown that a three layer ANN with sigmoid transfer functions can map any function of practical interest, a three layer neural network model is used in the present work. This network consists of 9 input nodes, a number of hidden nodes, and an output variable representing the beta transus temperature. The 44 dataset used was divided into two groups, each containing 22 input-output data pairs, for model training and model verification respectively.

There is no short cut to determining the number of hidden nodes, but through observing the performance of each model. The number of hidden nodes used here is from 2 to 10. Training process has been performed for each model. The performance of a model can be evaluated by its training error and testing error. Training of the neural networks stops when the verification error begins to increase [17]. The training error decreases as the number of hidden nodes increases. However, the complexity of the model also increases with the number of hidden units. A high degree of complexity may not be justified, and in an extreme case, the model may meaninglessly attempt to fit the noise in the experimental data. In circumstances where two models give similar results over the known data set, the more probable model would be predicted to be that which is simpler.

There are nine models tested in the current work, and results show that the model with 5 hidden nodes is of the best performance (model 9-5-1). Statistical analysis of the 9-5-1 model, compared with another model 9-10-1 (10 hidden nodes), is listed in Table 3, where Mean error and Error deviation were calculated using fomula (1) and (2) as well. Figures 4 and 5 illustrate the performance of this model on training data and verification data.

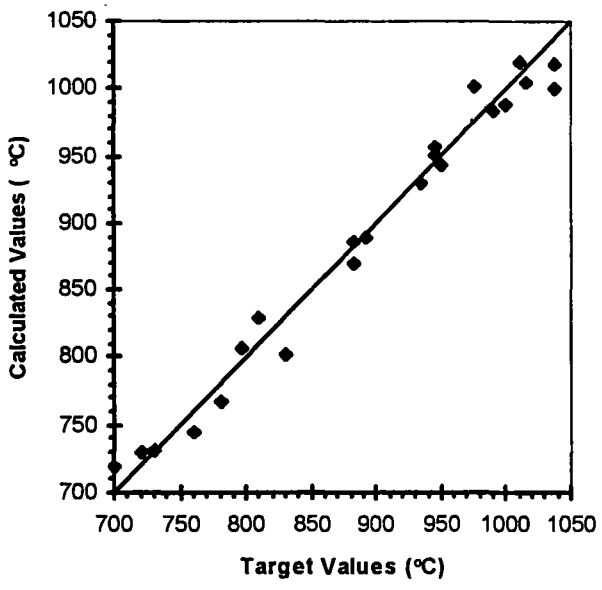

Figure 4 Performance of 9-5-1 model on training data

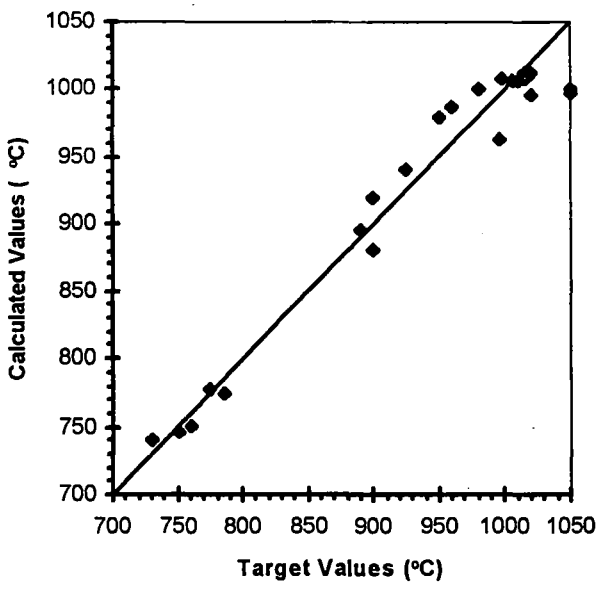

Figure 5 Performance of 9-5-1 model on verification data

Table 3 Statistical analysis of model 9-5-1 and 9-10-1 (β-transus in °C)

Data analysis	Experimental data		9-5-1 model		9-10-1 model	
	Mean value	Data S.D.	Mean error	Error deviation	Mean error	Error deviation
Training data	892	110	-2.1	16	-1.7	19
Verification data	931	106	-3.3	22	-0.3	24
Whole dataset	912	108	-2.7	19	-0.7	22

3.3.2. Beta transus prediction

The 9-5-1 neural network model was used to do β-transus prediction for five titanium alloys, which had not been used in training and verification. Therefore the results can give some indication of the performance of this neural network model. The results are shown in Table 4, compared with results from Thermo-Calc calculation. It should be noted that TB1, TB2 are beyond the concentration range limited by Thermo-Calc, and alloy specification instead of real composition were used for TB1, TB2 and TB3. However, the performance of a neural network model should be tested with a large amount of data rather than just a few cases.

Table 4 Modelling results of 9-5-1 neural network model (β-transus in °C)

Alloy designation	Experimental data	Using 9-5-1 model		Using Thermo-Calc	
		Result	Error	Result	Error
TB1 (Ti-3Al-3Mo-11Cr)	765	735	30	806	-41
TB2 (Ti-3Al-5Mo-5V-8Cr)	750	739	11	784	-34
TB3 (Ti-3.5Al-10Mo-8V-1Fe)	755	775	-20	743	12
Ti-13V-2.7Al-7Sn-2Zr	765	774	-9	776	-11
Ti-5Al-1Sn-1V-1Zr-0.8Mo	980	989	-9	980	0

3.3.3. Phase diagram calculation of Ti-Al and Ti-Mo

The influences of Al and Mo on beta transus temperature have also been quantified using the 9-5-1 model, compared with the results from Thermo-Calc calculation. Results are shown in Figure 6 and Figure 7, where experimental data are also illustrated [11]. As O and Fe are always present, their contents were treated as 0.1% and 0.2%, while using Thermo-Calc to do the calculation. It can be seen that results of both models agree with

the experimental data reasonably well, especially when their concentrations are no more than 5%wt. However, the error from either method increases when the element content is out of its compositional limitation. This phenomenon is very obvious when Al is over 7%wt for the case using 9-5-1 model to calculate Ti-Al diagram. Attempt was also taken to imitate the influence of O on the beta transus temperature. Whereas the Thermo-Calc calculation can give accurate results and neural network model cannot fulfill the job as O, C, N were not taken into account in training. It can also be seen that for both Ti-Al and Ti-Mo binary phase diagrams calculation, Thermo-Calc can generate more accurate results than using ANNs modelling. This might be attributed to the wide validation of Ti-Data database during its creation and development phases using some well-studied and commonly-used phase diagrams especially binary phase diagrams.

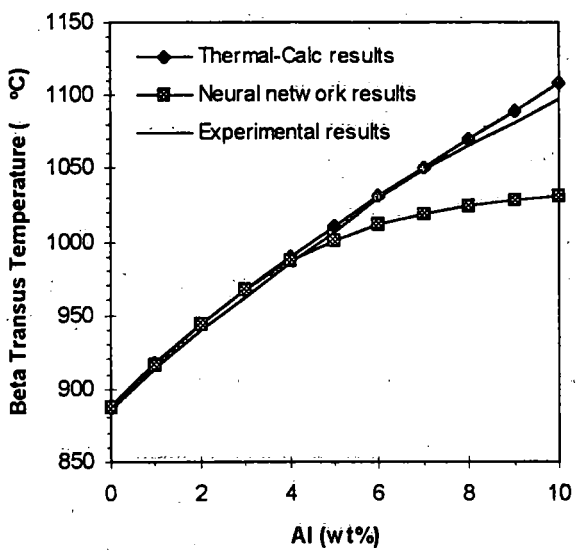

Figure 6 Comparison of different models with experimental results for Ti-Al system

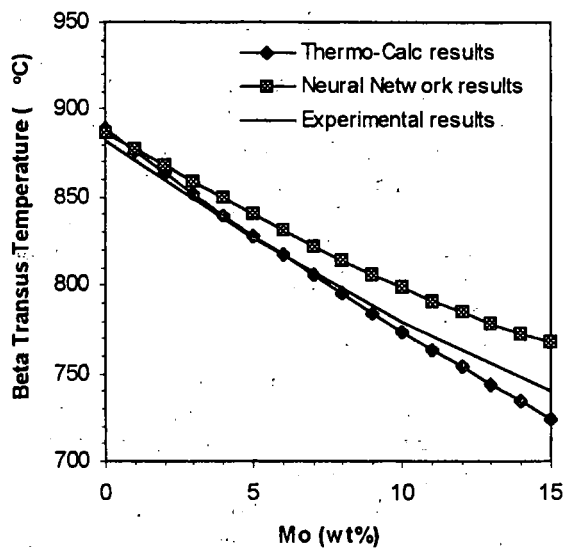

Figure 7 Comparison of different models with experimental results for Ti-Mo system

4. CONCLUSIONS

Two different methods have been used to model the beta transus temperature of titanium alloys. One is based on thermodynamic calculation, using the Thermo-Calc package. The other is artificial neural networks modelling, which takes beta transus as an implicit function of chemical composition. Results of both methods agree with the experimental results very well. The well-trained neural network model has also been used to predict the beta transus temperature of new alloys with good performance. Moreover, influences of alloy element Al and Mo on the beta transus temperature in binary systems have been modelled. However, both methods have their own compositional limitations for each element, which restrains their applications.

ACKNOWLEDGEMENT

Much appreciation is given to Dr. A. Hunter, Trajan Software Ltd, Co. Durham, U.K., for useful discussion and using his Trajan2.1 Shareware software. The authors also appreciate Dr. A.F. Wilson, TIMET, U.K., for the useful discussion and Dr. Y.Q. Zhao, Titanium Alloy Research Centre, Xi'an, China for his information on some titanium alloys. Meanwhile, particular thanks from Z. Guo to Dr. J.J. McKeown, School of Civil Engineering, The Queen's University of Belfast, U.K., for his kindly tutorials on artificial neural networks.

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Appendix An introduction to Ti-Data database

Ti-Data is a database created with specific aim of allowing phase diagram calculations to be performed for multi-component, conventional Ti-alloys. It contains most of the elements that are currently used in Ti-alloys. Moreover, it has been extensively validated against commercially useful alloys. Ti-Data contains the following elements:

Ti-Al-Cr-Fe-Mo-Nb-Si-Sn-Ta-V-Zr-C-O-N-B

The phases which are included in the database are:

Liquid, BCC(β), HCP(α), Laves_C14, Laves_C15, $TiFe_2B_2$, Ti_5Si_3, TiZrSi, α_2-Ti_3Al, TiB, TiB_2, M(C,N), SiC, Ti_2N

It should also be noted that this database has been designed for use with conventional α/β-type Ti-alloys, and it has been validated in the compositional spectrum associated with such alloys. As such some compositional limitations should be recognised when using the database. These are stated for each element below:

Ti >75%wt	Al < 8%wt	Cr < 5%wt	Fe < 3%wt
Si < 0.5%wt	Sn < 5%wt	C < 0.08%wt	O < 0.3%wt
N < 0.04%wt	B < 0.05%wt		

Mo, Nb, Ta, V, Zr: Total levels of these elements in titanium alloys should not usually exceed 20%wt with maximum levels of individual additions not exceeding 15%.