Development of Thermodynamic Description of a Pseudo-Ternary System for Multicomponent Ti64 Alloy

F. Zhang, S.-L. Chen, Y.A. Chang, N. Ma and Y. Wang

(Submitted October 13, 2006)

A method is presented to obtain a thermodynamic description of a multicomponent alloy system in terms of a pseudo-ternary formalism. In the present study, this method was applied to multicomponent Ti64 alloys with the "6" and "4" denoting the nominal 6 wt.% of Al and 4 wt.% of V in this class of Ti alloys. However these alloys, in practice, contain many other alloying elements such as O, C N, Fe, and H which exhibit appreciable effect on the thermodynamic properties of Ti64. The essence of this approach is to treat the multicomponent alloys as a pseudo-ternary Ti-Al$_x$-V$_y$, in which the apparent composition of Al$_x$ is the weighted summation of that of Al and those of the α-stabilizers in minor quantities such as O, C and N and that of V$_y$ is the weighted summation of that of V and those of the β stabilizing minor elements such as Fe and H. Three Ti64 alloys with slightly different chemistries were treated as pseudo-ternary alloys, and the β transus and β (and α) approach curves were calculated using this pseudo-ternary thermodynamic description. The calculated results were found to compare favorably with those calculated from a multicomponent thermodynamic database for titanium alloys. This study demonstrates that such a simplified thermodynamic description, when available, can be readily coupled with kinetic models for engineering applications. One example is to predict microstructure evolution of a multicomponent alloy when subjected to a specific heat treatment condition.

Keywords	CALPHAD, phase diagram, Phase-Field modeling

1. Introduction

It is well-known that the mechanical properties of an alloy depend on its microstructure, which is determined by the alloy chemistry, heat treatment, and processing conditions. If the correlation between them can be well-established, the desired microstructure and mechanical properties can be achieved through the optimization of alloy chemistry and processing conditions. However, establishing such a correlation is not

easy due to the fact that commercial alloys are usually multicomponent in nature and phase transformation and microstructural evolution processes are quite complex. Optimization of processing conditions for desired microstructure still depends largely on the traditional trial-and-error method. Recently, there has been an increasing effort in developing and integrating computational approaches so that the optimization process can be placed on a virtual prototyping basis to reduce the time and cost for the development of new alloys and modification of existing ones.[1] Among these modeling approaches, the Phase-Field method is well-known for its abilities of handling complex microstructures consisting of diffusionally and elastically interacting precipitates.[2-5] Theoretically, this method is able to handle multicomponent and multiphase alloys. However, quantitative modeling of multicomponent alloys by Phase-Field method requires that the fundamental model inputs to be linked with multicomponent thermodynamic and mobility databases.[6,7] This poses many difficult challenges. First of all, a direct coupling of the Phase-Field method with multicomponent thermodynamic calculation engine is not realistic at the moment because of millions of iterations of function calls. Second, direct implementation of the Gibbs energy functions of a multicomponent and multiphase system into the Phase-Field modeling is not easy since construction of a non-equilibrium free energy hypersurface needed by the Phase-Field method in a multidimensional space using these thermodynamic equilibrium Gibbs energies is not trivial. Finally, diffusivity data for many trace elements in the multicomponent alloys are unknown. The application of the Phase-Field method to commercial alloys is therefore hindered because of these challenges. For

F. Zhang, and **S.-L. Chen,** CompuTherm, LLC, 437 S. Yellowstone Dr., Ste. 217, Madison, WI 53719; **Y.A. Chang,** Department of Materials Science & Engineering, University of Wisconsin-Madison, 1509 University Ave., Madison, WI 53706; and **N. Ma** and **Y. Wang,** Department of Materials Science & Engineering, Ohio State University, 2041 College Rd., Columbus, OH 43221. Contact e-mail: Fan.Zhang@computherm.com

example, the existing work[7,8] treated commercial Ti64 alloy as a true ternary Ti-6wt.%Al-4wt.%V alloy.

In order to link thermodynamic calculation with kinetic models for multicomponent commercial alloys without confronting the above-mentioned difficulties, a simplified approach of obtaining a thermodynamic description of a multicomponent alloy system in terms of a pseudo-ternary formalism is presented in this article. This approach has been used to develop a pseudo-binary system for a nickel-based alloy,[9] and will be extended in this work for the development of a pseudo-ternary system for Ti64 alloy. Ti64 is presently the most widely used titanium alloy in the world, with most of its applications in aerospace industry. Even though, Ti64 denotes the nominal 6 wt.% of Al and 4 wt.% of V, commercial Ti64 alloy contains small amounts of Fe, O, C, N, H, and others which have significant effects on its phase equilibria and mechanical properties. For example, 0.1wt.% of O, C, N, or H can vary the β transus of Ti64 alloy by 20 °C or more. Higher contents of the O and N will increase the alloy strength; while lower contents of O and N will improve the ductility, fracture toughness, and stress-corrosion resistance. It is therefore essential to include all these elements in the simulation of microstructure and mechanical properties of Ti64 alloy. In this study, a thermodynamic description that has a similar format of that of the Ti-Al-V ternary but accounts for the effects of Fe, O, C, N, and H in the Ti64 alloy is developed. In the following, the formulation of such a pseudo-ternary system is presented followed by its application in the calculation of β transus and β (and α) approach curves for several Ti64 alloys with slightly different chemistries. The calculated results are compared with those calculated directly from a full multicomponent thermodynamic database.

2. Thermodynamic Description of a Pseudo-Ternary System for Ti64 Alloy

The Gibbs energy of α or β has the following format in the Ti-Al-V ternary system:

$$
\begin{aligned}
G^{\phi} = &\, x_{\text{Al}} \cdot G^{\phi}_{\text{Al}} + x_{\text{Ti}} \cdot G^{\phi}_{\text{Ti}} + x_{\text{V}} \cdot G^{\phi}_{\text{V}} \\
&+ RT(x_{\text{Al}} \cdot \ln x_{\text{Al}} + x_{\text{Ti}} \cdot \ln x_{\text{Ti}} + x_{\text{V}} \cdot \ln x_{\text{V}}) \\
&+ x_{\text{Al}} \cdot x_{\text{Ti}} \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{\text{Al}-\text{Ti}} (x_{\text{Al}} - x_{\text{Ti}})^{\ell} \\
&+ x_{\text{Ti}} \cdot x_{\text{V}} \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{\text{Ti}-\text{V}} (x_{\text{Ti}} - x_{\text{V}})^{\ell} \\
&+ x_{\text{Al}} \cdot x_{\text{V}} \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{\text{Al}-\text{V}} (x_{\text{Al}} - x_{\text{V}})^{\ell} \\
&+ x_{\text{Al}} \cdot x_{\text{Ti}} \cdot x_{\text{V}} \cdot L^{\phi,0}_{\text{Al}-\text{Ti}-\text{V}}
\end{aligned} \quad \text{(Eq 1)}
$$

where ϕ represents either the α or the β phase, x_i is the mole fraction of component i. G^{ϕ}_i represents the Gibbs energy of pure component i with ϕ structure; $L^{\phi,\ell}_{i-j}$ is binary interaction between i and j components, and when $n = 0$, it reduces to a regular solution model, $L^{\phi,0}_{\text{Al}-\text{Ti}-\text{V}}$ is the ternary interaction parameter, and $L^{\phi,\ell}_{i-j}$ and $L^{\phi,0}_{\text{Al}-\text{Ti}-\text{V}}$ are usually called model parameters, whose values are obtained by optimization

using experimental data. The Gibbs energy of α (or β) in the ternary system basically includes contributions from pure components (the first three terms), the ideal mixing term (the fourth term), binary interactions from the three constituent binaries, and ternary interaction (the last term). The model is relatively simple and straightforward.

The Gibbs energy expressions for these two phases in a multicomponent system are much more complicated. Assume that in addition to Al and V, we also consider Fe, O, N, C, and H in Ti64 alloy, the Gibbs energies of α and β can be described by a 2-sublattice compound-energy-formalism:[10,11] $(\text{Al},\text{Fe},\text{Ti},\text{V})_{f_1} : (\text{C},\text{H},\text{N},\text{O},\text{Va})_{f_2}$ as:

$$
\begin{aligned}
G^{\phi} = &\sum_{p,q} y^{\text{I}}_p \cdot y^{\text{II}}_q \cdot G^{\phi}_{p:q} \\
&+ RT \left(f_1 \sum_p y^{\text{I}}_p \cdot \ln y^{\text{I}}_p + f_2 \sum_q y^{\text{II}}_q \cdot \ln y^{\text{II}}_q \right) \\
&+ \sum_{p_1 \neq p_2} y^{\text{I}}_{p_1} \cdot y^{\text{I}}_{p_2} \cdot y^{\text{II}}_q \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{p_1-p_2-q} \left(y^{\text{I}}_{p_1} - y^{\text{I}}_{p_2} \right)^{\ell} \\
&+ \sum_{q_1 \neq q_2} y^{\text{I}}_p \cdot y^{\text{II}}_{q_1} \cdot y^{\text{II}}_{q_2} \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{p-q_1-q_2} (y^{\text{II}}_{q_1} - y^{\text{II}}_{q_2})^{\ell} \\
&+ \sum_{p_1 \neq p_2 \neq p_3} y^{\text{I}}_{p_1} \cdot y^{\text{I}}_{p_2} \cdot y^{\text{I}}_{p_3} \\
&\cdot (y^{\text{I}}_{p_1} \cdot L^{\phi,0}_{p_1-p_2-p_3} + y^{\text{I}}_{p_2} \cdot L^{\phi,1}_{p_1-p_2-p_3} + y^{\text{I}}_{p_3} \cdot L^{\phi,2}_{p_1-p_2-p_3})
\end{aligned} \quad \text{(Eq 2)}
$$

where p represents components Al, Fe, Ti, and V in the first sublattice, q represents C, H, N, O, and Va (Vacancy) in the second sublattice; y^{I}_p, and y^{II}_q represent the species concentrations of components p and q in sublattice I and II, respectively; $G^{\phi}_{p:q}$ is the Gibbs energy of the compound $p_{f_1}q_{f_2}$ whose value can be obtained from experimental determination if $p_{f_1}q_{f_2}$ is a stable compound, or by optimization using experimental data related to this phase if it is a hypothetical one. Recently, *ab initio* calculation has been used to obtain such a value for an unstable $p_{f_1}q_{f_2}$ compound. When q is Va, $G^{\phi}_{p:q}$ is the Gibbs energy of pure component p. L's are model parameters; f_1 and f_2 represent the fraction of sublattice site I and II, respectively, with $f_1/f_2 = 1/3$ for the β phase, and $f_1/f_2 = 1/0.5$ for the α phase. The Gibbs energy for the multicomponent α or β phase includes the Gibbs energies of pure components, stable or unstable compound phases, an entropy term assuming ideal mixing of components on each sublattice, and interactions of six binaries and 28 ternaries. Obviously, the Gibbs energy expressions for the α and β phases in the multicomponent Ti64 alloy are much more complicated than those in the Ti-Al-V ternary system. It would be extremely difficult to implement such a Gibbs energy function into Phase-Field models. In the following we demonstrate how to simplify the calculations by using a pseudo-ternary formulation.

For the modeling of phase transformation and microstructural evolution of Ti64 alloy, the key input parameter from thermodynamic calculation is the chemical driving force of forming α from β which is represented by the relative position of the Gibbs energy surface of α and β in the multi-dimensional space. The idea is therefore to develop a

thermodynamic description that can be used to calculate the chemical driving force of multicomponent commercial Ti64 alloy in terms of a pseudo-ternary formalism. Since it is difficult to explicitly represent the chemical driving force as a function of temperature and composition, other thermodynamic properties must be used to reflect the variation of the chemical driving force. Since equilibrium phase amounts of α and β are also determined by the relative position of their Gibbs energy surfaces, the β transus (the temperature at which β starts to transform to α) and β (or α) approach curve (equilibrium fraction of the β (or α) phase as a function of temperature) are therefore selected as target functions in the development of such a pseudo-ternary system. In this description, the effects of Fe, O, N, C, and H are accounted for by assuming that O, N, and C are Al-like, and Fe and H are V-like, which is based on the fact that O, N, and C are all α stabilizers like Al, while Fe and H are β stabilizers like V.

For the thermodynamic description of the pseudo-ternary system, the Gibbs energies of α and β will adopt the same format of Eq 1 as shown below:

$$G^\phi = x_{Al_x} \cdot G^\phi_{Al} + x_{Ti_b} \cdot G^\phi_{Ti} + x_{V_y} \cdot G^\phi_V$$
$$+ RT(x_{Al_x} \cdot \ln x_{Al_x} + x_{Ti_b} \cdot \ln x_{Ti_b} + x_{V_y} \cdot \ln x_{V_y})$$
$$+ x_{Al_x} \cdot x_{Ti_b} \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{Al_x-Ti_b}(x_{Al_x} - x_{Ti_b})^\ell$$
$$+ x_{Ti_b} \cdot x_{V_y} \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{Ti_b-V_y}(x_{Ti_b} - x_{V_y})^\ell$$
$$+ x_{Al_x} \cdot x_{V_y} \cdot \sum_{\ell=0}^{n} L^{\phi,\ell}_{Al_x-V_y}(x_{Al_x} - x_{V_y})^\ell$$
$$+ x_{Al_x} \cdot x_{Ti_b} \cdot x_{V_y} \cdot L^{\phi,0}_{Al_x-Ti_b-V_y} \quad \text{(Eq 3)}$$

In the above equation, we still use the Gibbs energies of pure components Al, Ti, and V to describe the reference state. The binary and ternary interaction parameters are different from those of the true ternary Ti-Al-V system since they are now interactions between the pseudo-binaries and the pseudo-ternary. The mole fraction, x_{Al_x}, is now the weighted summation of those of Al, O, C, and N, x_{V_y} the weighted summation of those of V, Fe, and H, and x_{Ti_b} is the balance, i.e.,

$$x_{Al_x} = x_{Al} + \lambda_O \cdot x_O + \lambda_C \cdot x_C + \lambda_N \cdot x_N \quad \text{(Eq 4)}$$

$$x_{V_y} = x_V + \lambda_{Fe} \cdot x_{Fe} + \lambda_H \cdot x_H \quad \text{(Eq 5)}$$

in which λ_i's are the weighing factors used for calculating the Al-equivalent content and V-equivalent content. In order to determine these factors, industrial experiences and semi-empirical relations have to be used. Since it is more convenient for the industry to use weight fraction or weight percent instead of mole fraction, Eq 4 and 5 can be converted to weight fraction as:

$$w_{Al_x} = w_{Al} + \lambda_O \frac{M_{Al}}{M_O} w_O + \lambda_C \frac{M_{Al}}{M_C} w_C + \lambda_N \frac{M_{Al}}{M_N} w_N \quad \text{(Eq 6)}$$

$$w_{V_y} = w_V + \lambda_{Fe} \frac{M_V}{M_{Fe}} w_{Fe} + \lambda_H \frac{M_V}{M_H} w_H \quad \text{(Eq 7)}$$

where w_i and M_i represent the weight fraction and the atomic weight of component i, respectively. An assumption of $M_{Al_x} = M_{Al}$ and $M_{V_y} = M_V$ is used to derive Eq 6 and 7 for simplicity. This is reasonable since the amounts of O, C, N, Fe, and H are very small compare to those of Al and V.

In the handbook for titanium alloys edited by Boyer et al.,[12] Al- and Mo-equivalent formats (in wt.%) are given for variety of elements in different classes of titanium alloys, focussing primarily on the strengthening effects. For example, a factor of 10 is given for O, 2.5 for Fe, 0.667 for V, and so on to calculate the Al- and Mo-equivalent contents for Ti64. On the other hand, a factor of 1.69 is used for O by a semi-empirical relation[13] for the calculation of β transus of Ti64. Due to the large variation of these equivalent factors, selection of their values becomes a difficult task. However, since the purpose of the present work is to develop a pseudo-ternary description of Ti64 for the kinetic simulation of microstructural evolution, the primary concerns are the β transus temperature and β approach curve which are directly related to the chemical driving force of β/α transformation. Even though the effect of O, C, N, and H on the β transus can be 10-20 times large as that of Al and V, we cannot use such large factors because we would overestimate the effects of these minor additions on the β approach curve. In order to optimize the description of both β transus temperature and β approach curve by the pseudo-ternary system, the following equivalent factors are used:

$$\lambda_O \frac{M_{Al}}{M_O} = 2 \quad \text{(Eq 8a)}$$

$$\lambda_C \frac{M_{Al}}{M_C} = 5 \quad \text{(Eq 8b)}$$

$$\lambda_N \frac{M_{Al}}{M_N} = 5 \quad \text{(Eq 8c)}$$

$$\lambda_{Fe} \frac{M_V}{M_{Fe}} = 1.5 \quad \text{(Eq 8d)}$$

$$\lambda_H \frac{M_V}{M_H} = 25 \quad \text{(Eq 8e)}$$

In other words, these factors in Eq 8(a) to (e) are chosen according to weight fraction (or percent). It is also noticed that,

$$M_{Al} \approx 2M_O \approx 2M_C \approx 2M_N \quad \text{(Eq 9)}$$

$$M_V \approx M_{Fe} \approx 50M_H \quad \text{(Eq 10)}$$

This gives:

$$\lambda_O = 1 \quad \text{(Eq 11a)}$$

$$\lambda_C = 2.5 \quad \text{(Eq 11b)}$$

$$\lambda_N = 2.5 \quad \text{(Eq 11c)}$$

$$\lambda_{Fe} = 1.5 \qquad \text{(Eq 11d)}$$

$$\lambda_H = 0.5 \qquad \text{(Eq 11e)}$$

Substituting Eq 8(a) to (e) and Eq 11(a) to (e) into Eq 4 through 7, we have:

$$x_{Al_x} = x_{Al} + x_O + 2.5x_C + 2.5x_N \qquad \text{(Eq 12)}$$

$$x_{V_y} = x_V + 1.5x_{Fe} + 0.5x_H \qquad \text{(Eq 13)}$$

$$w_{Al_x} = w_{Al} + 2w_O + 5w_C + 5w_N \qquad \text{(Eq 14)}$$

$$w_{V_y} = w_V + 1.5w_{Fe} + 25w_H \qquad \text{(Eq 15)}$$

The alloy composition of a pseudo-ternary system can then be easily calculated using Eq 12 and 13 if mole fraction (or percent) is used, and Eq 14 and 15 if weight fraction (or percent) is used.

It should be pointed out that, even though the entropy contributions of the interstitial elements are different from those of the substitutional ones, these effects are considered to be taken into account approximately by the empirical equivalent factors.

3. Results and Discussions

To validate the pseudo-ternary description of Ti64 formulated above, calculations are carried out using this description and compared with those standard calculations by **Pandat**[14] and a full multicomponent thermodynamic database for titanium alloys, **PanTi** developed at CompuTherm.[15] This database has been tested by a large number of titanium alloys, and two examples are shown in Fig. 1 and 2. Figure 1 shows comparison between the calculated and measured β transus temperatures for 150 heats. Good agreement is obtained for most of the heats. The sources of causing the differences between calculations and measurements have been discussed by Zhang et al.,[15] and will not be repeated here. Figure 2 shows the calculated β approach curve for one Ti64 heat which agrees well with the experimental data.[16]

The thermodynamic description of the pseudo-ternary system is first applied to a Ti64 alloy with the following chemistry: Ti-6.624Al-4.096V-0.194Fe-0.1855O-0.0065N-0.02C-0.0044H in wt.%, or Ti-11.14Al-3.65V-0.1576Fe-0.5262O-0.0211N-0.0756C-0.1981H in at.%. According to Eq 12-15, this is equivalent to a pseudo-ternary alloy with the chemistry of: Ti-7.1275Al$_x$-4.497V$_y$ (wt.%) or Ti-12.017Al$_x$-4.0159V$_y$ (at.%). Three pairs of α approach and β approach curves are shown in Fig. 3. The solid lines are calculated by using multicomponent thermodynamic database **PanTi**[15] for the full multicomponent chemistry given above. The dashed lines are calculated for the pseudo-ternary alloy chemistry, but using the **true** Ti-Al-V database. The circle symbols are calculated for the same pseudo-ternary alloy chemistry while using the thermodynamic description of the pseudo-ternary system developed in this study, i.e., using the adapted values of interaction parameters given in Eq 3 instead of those in Eq 1. It is
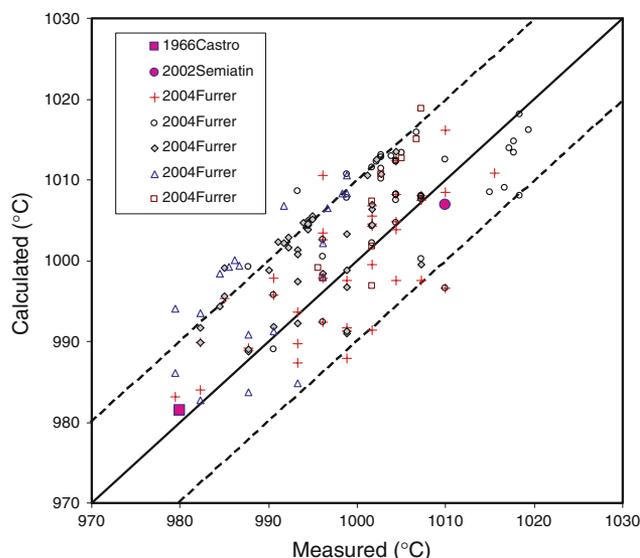
Fig. 1 Comparison between predicted and observed β transus for more than 150 Ti64 alloys. Calculations are carried out with **Pandat** software and **PanTi** database developed at CompuTherm
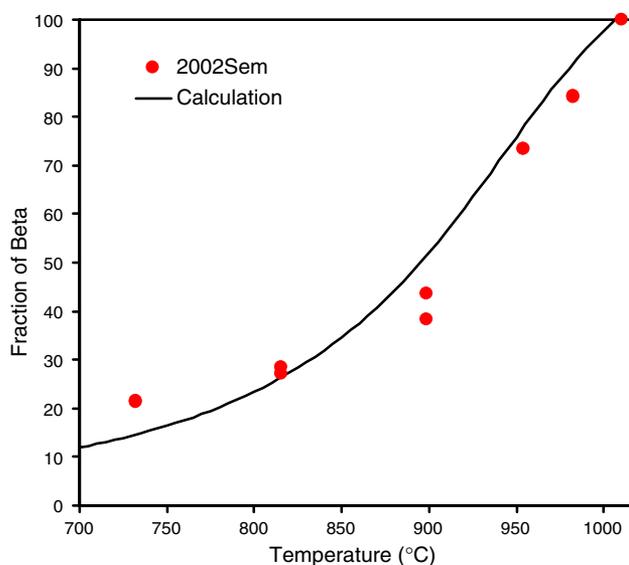
Fig. 2 β approach curve calculated for one Ti64 alloy (Ti-6.42Al-4.2V-0.14Fe-0.004H-0.017C-0.005N-0.19O in wt.%) with experimental data from Semiatin[16]

clearly seen that the β transus, and β and α approach curves calculated using the pseudo-ternary description agree well with those obtained from the full multicomponent thermodynamic database, while the ones calculated by the **true** Ti-Al-V ternary database show significant deviations. One can conclude from Fig. 3 that the Ti64 alloy with the following chemistry: Ti-6.624Al-4.096V-0.194Fe-0.1855O-0.0065N-0.02C-0.0044H (wt.%) can be described as a pseudo-ternary alloy with the chemistry of Ti-7.1275Al$_x$-4.497V$_y$ (wt.%) or Ti-12.017Al$_x$-4.0159V$_y$ (at.%) using the pseudo-ternary database developed in this work.
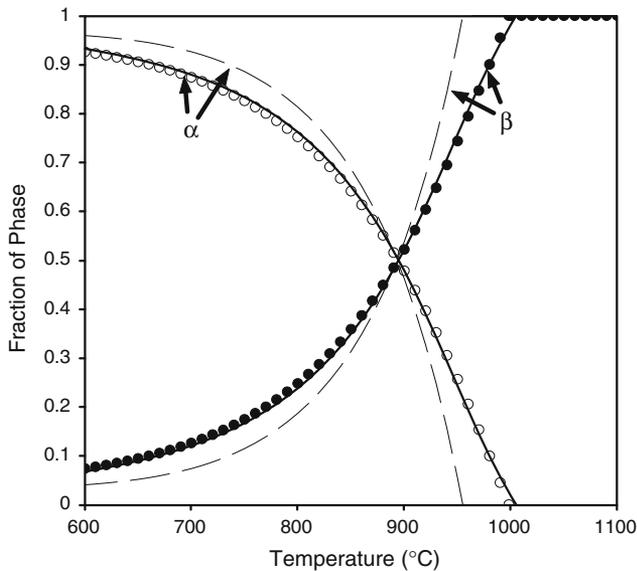
Fig. 3 Calculated α and β approach curves for Ti64 alloy with the chemistry of: Ti-6.624Al-4.096V-0.194Fe-0.1855O-0.0065N-0.02C-0.0044H (wt.%). The solid lines are calculated using the multicomponent thermodynamic database **PanTi** for the chemistry given above. The dashed lines are calculated for the pseudo-ternary chemistry: Ti-7.1275Al$_x$-4.497V$_y$ (wt.%) using the **true** Ti-Al-V ternary database, and the solid and open circles are calculated for the same ternary chemistry but using the pseudo-ternary database developed in this study
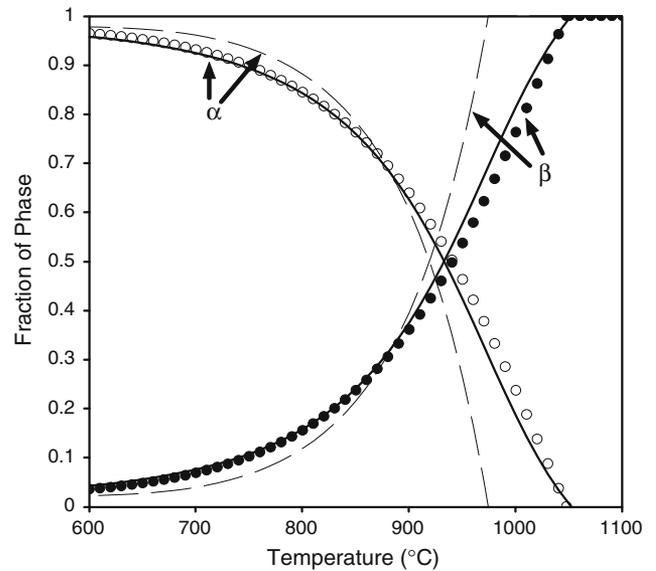
    If this database can only be applied to this particular Ti64 chemistry, it is not attractive due to the fact that commercial Ti64 alloy has a range of chemistry. Based on the titanium alloy handbooks and published literature,[12] the following composition range is found to cover most of the Ti64 chemistries: Ti-5.5 ~ 6.75Al-3.5 ~ 4.5V-0.15 ~ 0.25Fe-0.13 ~ 0.23O-0.005 ~ 0.02N-0.01 ~ 0.05C-0.002 ~ 0.008H (wt.%). To test if the thermodynamic description of the pseudo-ternary would work in this composition range, two extreme chemistries are chosen for calculations: one maximizes all the α stabilizers and minimizes the β stabilizers, and the other the reverse case. The two chemistries are: Ti-6.75Al-3.5V-0.15Fe-0.23O-0.02N-0.05C-0.002H (wt.%), and Ti-5.5Al-4.5V-0.25Fe-0.13O-0.005N-0.01C-0.008H (wt.%). Calculated results for these two chemistries are shown in Fig. 4 and 5. Surprisingly, the database for the pseudo-ternary system works very well for these two extreme chemistries! This indicates that the pseudo-ternary description developed in this study can be applied to any Ti64 alloy whose chemistry locates within the specification range: Ti-5.5 ~ 6.75Al-3.5 ~ 4.5V-0.15 ~ 0.25Fe-0.13 ~ 0.23O-0.005 ~ 0.02N-0.01 ~ 0.05C-0.002 ~ 0.008H (wt.%) or Ti-9.33 ~11.33 Al-3.11 ~ 4.04V-0.12 ~ 0.2Fe-0.37 ~ 0.65O-0.016 ~ 0.065N-0.038 ~ 0.188C-0.09 ~ 0.36H (at.%). Beyond this composition range, some model parameters for the pseudo-ternary description may need to be adjusted.

    It should be noted that the pseudo-ternary description developed in this study is optimized for calculating β transus, and β and α approach curves. This description can

Fig. 4 Calculated α and β approach curves for Ti64 alloy with the chemistry of: Ti-6.75Al-3.5V-0.15Fe-0.23O-0.02N-0.05C-0.002H (wt.%). Explanations for the lines and symbols are the same as those in Fig. 3. The corresponding pseudo ternary chemistry is: Ti-7.56Al-3.775V (wt.%)

be used to calculate the chemical driving force that are most relevant to kinetic modeling of α/β phase transformation and microstructural evolution. For the calculation of other thermodynamic properties, such as the equilibrium phase compositions at given temperatures, the full multicomponent thermodynamic database should be used.

4. Summary

    There is a great demand of modeling capabilities in predicting the correlation between mechanical properties, microstructure, alloy chemistry, and processing conditions for commercial alloys. In order to establish such a correlation, model integration plays a key role. For example, in the prediction of processing-microstructure relationship, kinetic modeling tools, such as Phase-Field method, must be integrated with thermodynamic modeling tools. Such integration is challenged by the complexity of multicomponent thermodynamics of commercial alloys. As an attempt of making such integration attractive, an approach of using pseudo-ternary to represent multicomponent alloy is presented and a thermodynamic database for a pseudo-ternary system is developed for Ti64 alloy. This database is tested against the full multicomponent thermodynamic database for titanium alloys and is found to work well for any Ti64 alloy whose chemistry is within the range of: Ti-5.5 ~ 6.75Al-3.5 ~ 4.5V-0.15 ~ 0.25Fe-0.13 ~ 0.23O-0.005 ~ 0.02N-0.01 ~ 0.05C-0.002 ~ 0.008H (wt.%), which corresponds to: Ti-9.33 ~ 11.33Al-3.11 ~ 4.04V-0.12 ~ 0.2Fe-0.37 ~ 0.65O-0.016 ~ 0.065N-0.038 ~ 0.188C-0.09 ~ 0.36H (at.%). For an alloy beyond this composition range, further
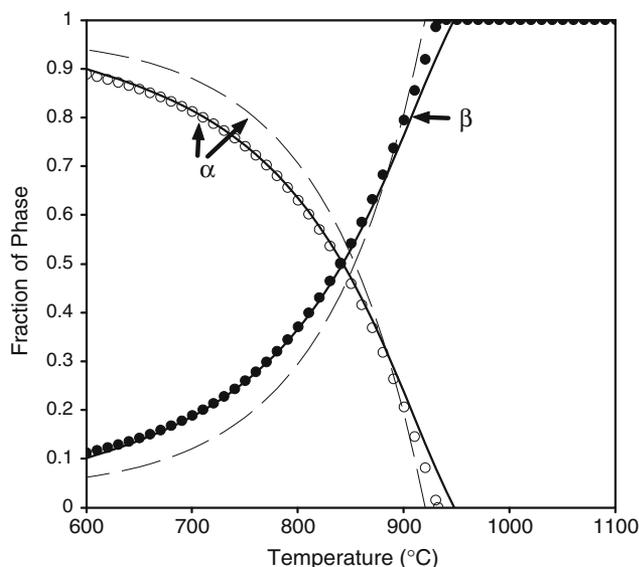
Fig. 5 Calculated α and β approach curves for Ti64 alloy with the chemistry of: Ti-5.5Al-4.5V-0.25Fe-0.13O-0.005N-0.01C-0.008H (wt.%). Explanations for the lines and symbols are the same as those in Fig. 3. The corresponding pseudo ternary chemistry is: Ti-5.835Al-5.075V (wt.%)

validation is needed. To carry out calculations using this pseudo-ternary database, one must first simplify the multi-component to a pseudo-ternary Ti-Al$_x$-V$_y$. The composition of the pseudo-ternary alloy can be calculated by Eq 12 and 13 if using mole fraction or atomic percent, or Eq 14 and 15 if weight fraction (or percent) is used. Even though only β transus, and β and α approach curves are calculated using the pseudo-ternary description, this description can be used to calculate the chemical driving force of α/β phase transformation for multicomponent Ti64 alloy. Furthermore, the pseudo-ternary description provides a simple Gibbs free energy function for Phase-Field simulation, which makes it possible to simulate the phase transformation and micro-structural evolution of commercial Ti64 alloy that account for variations in alloy chemistry. The approach developed in this study can also be used for the development of pseudo-binary or ternary descriptions of other commercial alloys. This may open an avenue for many potential industrial applications.

References

1. Y. Wang, N. Ma, Q. Chen, F. Zhang, S.L. Chen, and Y.A. Chang, *JOM*, 2005, **57**(9), p 32-39
2. Y. Wang, L.Q. Chen, and A.G. Khachaturyan, *Computer Simulation in Materials Science Nano/Meso/Macroscopic Space and Time Scales*, Kluwer Academic Publishers, 1996
3. Y. Wang and L.Q. Chen, *Simulation of Microstructural Evolution Using the Field Method*, John Wiley & Sons. Inc., 2000
4. A. Karma, *Phase-Field Methods*, Elsevier, Oxford, 2001
5. L.Q. Chen, *Annu. Rev. Mater. Res*, 2002, **32**, p 113
6. C. Shen, J.P. Simmons, K. Wu, and Y. Wang, *Materials Design Approaches and Experiences*, TMS, 2001, p 57-74
7. Q. Chen, N. Ma, K. Wu, and Y. Wang, *Scripta Mater.*, 2004, **50**, p 471-476
8. N. Ma, A. Kazaryan, S.A. Dregia, and Y. Wang, *Acta Mater.*, 2004, **52**, p 3869
9. B. Wang et al., in preparation (2006)
10. I. Ansara, *Int. Metals Rev.*, 1979, **24**, p 20-53
11. B. Sundman and J. Agren, *J. Phys. Chem. Solids*, 1981, **42**, p 297-301
12. R. Boyer, G. Welsch, and E.W. Collings (Eds.), *Materials Properties Handbook: Titanium Alloys*, ASM International, Materials Park, OH 44073-0002, 1994
13. R. Boyer, *Private communication* (2006)
14. S.L. Chen, F. Zhang, S. Daniel, F.-Y. Xie, X.-Y. Yan, Y.A. Chang, R. Schmid-Fetzer, and W.A. Oates, *JOM*, 2003, **55**(12), p 48-51
15. F. Zhang, F.-Y. Xie, S.-L. Chen, Y.A. Chang, D. Furrer, and V. Venkatesh, *J. Mater. Engineer. Perform.*, 2005, **14**(6), p 717-721
16. S.L. Semiatin, F. Montheillet, G. Shen, and J.J. Jonas, *Metall. Mater. Trans. A.*, 2002, **33**(8), p 2719-2727
17. D. Furrer, Private Communication, 2004
18. R. Castro and L. Seraphin, *Mem. Sci. Rev. Met.*, 1966, **63**, p 1025-1058