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Thermodynamic modeling of the Ti-Nb-Sn system and its preliminary applications in aging precipitation and solidification simulations

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Abstract

Gasping the thermodynamic and phase diagram of the materials being studied is essential for further guiding the development process, like composition design, heat treatment optimization and so on. Nb and Sn are common alloying elements in Ti-based biomedical alloys. In this work, the Ti-Nb-Sn system has been thermodynamically assessed based on experimental phase equilibria. A self-consistent thermodynamic description for the Ti-Nb-Sn system including two ternary compounds Ti3Nb3Sn2 and Ti5NbSn has been obtained. Based on the comparison between the calculated and experimental phase equilibria, the reliability of the presently obtained thermodynamic description has been verified. The influence of Nb and Sn contents on the precipitation temperature and amount of hcp α-Ti phase in bcc β-(Ti, Nb) has been investigated based on thermodynamic calculations. Results show that the increase of Nb or Sn content in Ti-based alloys would significantly reduce the precipitation amount and transformation temperature of hcp α-Ti phase in bcc β-(Ti, Nb) and the influence of Nb content is more effective than that of Sn. The solidified phases in several as-cast alloys have been thermodynamically predicted based on Scheil solidification simulations. The presently developed thermodynamic description of the Ti-Nb-Sn system can serve as a sub-ternary one in the thermodynamic database for multicomponent Ti-based biomedical alloys.

1. Introduction

Due to the desirable properties such as similar Young’s modulus to human bones, high strength, corrosion resistance behavior and good biocompatibility, titanium-base alloys have been extensively applied in biomedical applications [1–3]. In order to enhance the biomedical properties of titanium-base alloys, alloying elements like Nb, Sn, Zr, Ta, Mo have been reported to obtain promising properties [2–5]. It is reported that the alloying of Nb and Sn in Ti-based alloys can significantly increase strength and reduce elastic modulus to human bones’ level without increasing the martensitic transformation temperature [6, 7]. It is well known that the microstructure of a material is the ‘fingerprint’ of its mechanical properties. Therefore, studying the thermodynamic behavior of each phase in alloys is extremely important for materials development.

Initially, Ti-based alloys may present a microstructure composed of bcc β-stabilizer by rapid cooling. Subsequently, such alloys are subjected to aging treatment in order to obtain hcp α-Ti precipitates [8]. Thus, an optimal combination of properties corresponding to the strengthening precipitates can be obtained through the design of alloying composition and aging heat treatment. Nevertheless, the cost of experiment-only attempts is large. CALPHAD technique has been proven to be a powerful and useful tool to predict the phase stabilities and phase transformations [9], which can provide a strong theoretical basis. However, the thermodynamic modeling of the Ti-Nb-Sn system has not been established.

Consequently, the aim of this work is to critically evaluate the reported experimental phase equilibria, thermodynamically model the Ti-Nb-Sn system, study the influence of Nb and Sn content on the phase

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transformation of hcp $\alpha$-Ti phase and bcc $\beta$-(Ti, Nb), and finally analyze as-cast microstructures through Scheil solidification simulations.

2. Experimental information

Table 1 shows the symbols for the phases and the crystal structure information in the Ti-Nb-Sn ternary system, for facilitating reading.

The experimental information for the sub-binary systems has been critically reviewed in previous works [10–14], which will not be repeated here. The recent evaluations of the Ti-Nb [12], Ti-Sn [13] and Nb-Sn [14] binary systems are considered to be reliable and thus accepted in the present assessment of the Ti-Nb-Sn ternary system. Figure 1 shows the presently calculated phase diagrams of the Ti-Nb, Ti-Sn and Nb-Sn systems, using the thermodynamic parameters in [12–14].

The experimental phase diagram of the Ti-Nb-Sn system mainly comes from the contributions by Wang et al [10, 11]. Using XRD, SEM and EPMA techniques, the isothermal sections of the Ti-Nb-Sn system were constructed based on 15 equilibrium alloys at 973 K [10] and 23 equilibrium alloys at 1173 K [11]. Two ternary compounds were detected in the Ti-Nb-Sn system with one compound, $\text{Ti}_3\text{Nb}_3\text{Sn}_2$, at 973 K [10] and two compounds, $\text{Ti}_3\text{Nb}_2\text{Sn}_2$ and $\text{Ti}_2\text{NbSn}$, at 1173 K [11]. The crystal structure of $\text{Ti}_3\text{Nb}_2\text{Sn}_2$ was reported to be the same as that of Nb3Sn in the Nb-Sn binary boundary [10, 15]. $\text{Ti}_3\text{NbSn}$ was initially reported by Wang et al [11], however, without the crystal structure information. For the isothermal section at 973 K, 3 three-phase equilibria, all involving the ternary compound $\text{Ti}_3\text{Nb}_3\text{Sn}_2$, and 5 two-phase regions were experimentally detected [10]. The compositions of $\alpha$-Ti, $\beta$-(Ti, Nb), $\text{Ti}_3\text{Sn}$, $\text{Nb}_3\text{Sn}$ and $\text{Ti}_3\text{Nb}_2\text{Sn}_2$ were proposed based on EPMA results. For the isothermal section at 1173 K, 4 three-phase equilibria, involving $\text{Ti}_3\text{Nb}_2\text{Sn}_2$ and/or $\text{Ti}_2\text{NbSn}$, and 11 two-phase regions were determined [11]. Moreover, the binary compounds at Ti-Sn and Nb-Sn boundaries were detected to have significant solubilities along with nearly iso-concentration of Sn.

3. Thermodynamic models

The Gibbs energy expressions of pure Ti, Nb and Sn in the SGTE compilation of Dinsdale [16] are applied in this work. For the Ti-Nb binary system, the thermodynamic descriptions from Hari Kumar et al [17] and Saunders [12] have been reported in the literature. It is hard to say which one is better. However, the thermodynamic parameters reported by Saunders [12] have been widely applied in the development of thermodynamic databases for Fe-based alloys [18] and cemented carbides [19], and thus adopted in the present work. The first assessment of the Ti-Sn binary system is from the work by Hayes [20]. However, the later detected intermetallic compound, $\text{Ti}_2\text{Sn}_3$, was not considered in that work. Recently, another two reassessments of the Ti-Sn system were reported [13, 21], which show no major difference in the reproduce of experimental data. The more recent assessment from Yin et al [13] performed based on their own experimental data at the Sn-rich side was thus adopted in the present work. The Nb-Sn binary system was firstly assessed by Toffolon et al [22] and, soon later, reassessed by the same group [14] with the consideration of their experiments about the stability of the Nb3Sn phase. Most recently, Li et al [23] slightly modified the homogeneity range of the NbSn2 phase by considering the ternary Cu-Nb-Sn system. However, no substantial improvement has been made. As a result, the thermodynamic description reported by Toffolon et al [14] was adopted in the present work.

Table 1. Crystal structure data of phases in the ternary system.

| Phase  | Designation | Prototype | Personal Symbol | Space Group |
|--------|-------------|-----------|-----------------|-------------|
| $\alpha$-Ti | hcp         | Mg       | hP2             | P63/mmc     |
| $\beta$-Ti | bcc         | W        | cI2             | Im3m        |
| $\beta$-Nb | bcc         | W        | cI2             | Im3m        |
| $\text{Ti}_3\text{Sn}$ | $\text{Ti}_3\text{Sn}$ | $\text{Ni}_3\text{Sn}$ | hP8 | P4222 |
| $\beta$-Sn | bct          | $\beta$-Sn | —             | I41/amd     |
| $\alpha$-Sn | diamond | C(diamond) | cF8             | Fd3m        |
| $\text{Ti}_3\text{Sn}$ | $\text{Ti}_3\text{Sn}$ | $\text{Ni}_3\text{Sn}$ | hP6 | P63/mmc |
| $\text{Ti}_3\text{Sn}_3$ | $\text{Ti}_3\text{Sn}_3$ | $\text{Mn}_3\text{Sn}_3$ | hP16 | P63/mcm |
| $\text{Ti}_2\text{Sn}_3$ | $\text{Ti}_2\text{Sn}_3$ | $\text{Ti}_3\text{Sn}_3$ | oI44 | Immm |
| $\text{Ti}_3\text{Sn}_3$ | $\text{Ti}_3\text{Sn}_3$ | —         | oC40            | Cmca        |
| $\text{Nb}_2\text{Sn}$ | $\text{Nb}_2\text{Sn}$ | Cr$_3$Si | cp8             | Pm3n        |
| $\text{Nb}_3\text{Sn}_2$ | $\text{Nb}_3\text{Sn}_2$ | $\text{Ti}_3\text{Sn}_3$ | hp22 | P63/mmc |
| $\text{Nb}_3\text{Sn}_2$ | $\text{Nb}_3\text{Sn}_2$ | CuMg$_2$ | oF48            | Fd3d        |
| $\text{Ti}_2\text{Nb}_2\text{Sn}_2$ | $\text{Ti}_2\text{Nb}_2\text{Sn}_2$ | Cr$_3$Si | cp8             | Pm3n        |
The phases in the Ti-Nb-Sn system were modeled according to compound energy formalism \cite{24}. The current model of the Ti-Nb-Sn ternary system was derived from the recent assessments of the Ti-Nb \cite{12}, Ti-Sn \cite{13} and Nb-Sn \cite{14} binary systems. The solution phases, liquid, bcc, hcp, and bct, were described by substitutional solution model using the Redlich-Kister polynomial \cite{25}:

\[
0 \Delta G_m^\phi = \sum_i x_i \left( \frac{\partial G_i^\phi}{\partial y} \right) + RT \sum_i \left( x_i \ln x_i + \sum_{i,j>i} x_ix_j \sum_\nu L_{ij}^\nu (x_i - x_j)^\nu \right) + \sum_i \left( \frac{\partial G_i^\phi}{\partial \mu} \right)_{y=0} x_i y_i
\]

where \( x_i \) and \( x_j \) represent the molar fractions of elements (\( i, j = \text{Ti, Nb, Sn} \)). \( 0 \Delta G_i^\phi \) is the reference Gibbs energy of pure \( i \) at 298 K and 1 bar. \( L_{ij}^\nu \) is the interaction parameter from binary system. \( L_{ij}^\nu \) are ternary interaction parameters to be assessed in the current work.

According to the sublattice model \cite{26}, the intermetallic compounds, Ti3Sn, Ti2Sn, Ti5Sn3, Ti6Sn5, Ti2Sn3, Nb3Sn, NbSn2, are described by two-sublattice model, and three-sublattice model for Nb6Sn5. Based on the experimentally determined solubility range \cite{10,11}, a three-sublattice model is chosen for Ti3Nb3Sn2 in order to avoid the formation of a continuous phase among Ti3Nb3Sn2, Ti3Sn and Nb3Sn. The Ti3NbSn is also modeled by a three-sublattice model according to its solubility range because of the lack of crystallographic information. According to the experimental results \cite{10,11}, Ti3Nb3Sn2 and Ti3NbSn exhibit mainly the substitution between Ti and Nb atoms. Simply, both ternary compounds are treated as linear compounds with a constant Sn content. The thermodynamic models for Ti3Nb3Sn2 and Ti3NbSn are (Nb,Ti)3(Nb,Ti)3(Sn)2 and (Nb,Ti)3(Nb,Ti)3(Sn)1, respectively. Based on these models, the substitution between Ti and Nb can be directly described by endmembers accompanying no or less interaction parameters.

Taking a phase \( \phi \) modeled by (Nb, Sn, Ti)\((\text{Nb, Sn, Ti})\), for example, its Gibbs energy can be expressed as follows:

\[
0 \Delta G_m^\phi = \sum_i \sum_j y_i^\phi y_j^\phi G_{ij}^\phi + RT \left( a \sum_i y_i^\phi \ln y_i^\phi + c \sum_j y_j^\phi \ln y_j^\phi \right) + \sum_i \left( \frac{\partial G_i^\phi}{\partial y} \right)_{y=0} x_i y_i
\]

Figure 1. Sub-binary phase diagrams calculated using the reported thermodynamic parameters \cite{12–14}:
(a) Ti-Nb , (b) Ti-Sn and (c) Nb-Sn systems.
Table 2. Summary of the thermodynamic parameters in the Ti–Nb–Sn system.*

| Parameter | Value |
|-----------|-------|
| \( \Delta G_{\text{TiSn}}^{\text{f}} \) (J mol\(^{-1}\)) | 50180 |
| \( \Delta H_{\text{TiSn}}^{\text{f}} \) (J mol\(^{-1}\)) | 156400 |
| \( \Delta S_{\text{TiSn}}^{\text{f}} \) (J mol\(^{-1}\) K\(^{-1}\)) | 131656.9 |
| \( \Delta G_{\text{NbSn}}^{\text{f}} \) (J mol\(^{-1}\)) | 28670 |
| \( \Delta H_{\text{NbSn}}^{\text{f}} \) (J mol\(^{-1}\)) | 106258.9 |
| \( \Delta S_{\text{NbSn}}^{\text{f}} \) (J mol\(^{-1}\) K\(^{-1}\)) | 66258.9 |
| \( \Delta G_{\text{NbTi}}^{\text{f}} \) (J mol\(^{-1}\)) | 50180 |
| \( \Delta H_{\text{NbTi}}^{\text{f}} \) (J mol\(^{-1}\)) | 122344 |
| \( \Delta S_{\text{NbTi}}^{\text{f}} \) (J mol\(^{-1}\) K\(^{-1}\)) | 179808 |
| \( \Delta G_{\text{SnSn}}^{\text{f}} \) (J mol\(^{-1}\)) | 50180 |
| \( \Delta H_{\text{SnSn}}^{\text{f}} \) (J mol\(^{-1}\)) | 66258.9 |
| \( \Delta S_{\text{SnSn}}^{\text{f}} \) (J mol\(^{-1}\) K\(^{-1}\)) | 106258.9 |
| \( \Delta G_{\text{SnTi}}^{\text{f}} \) (J mol\(^{-1}\)) | 50180 |
| \( \Delta H_{\text{SnTi}}^{\text{f}} \) (J mol\(^{-1}\)) | 122344 |
| \( \Delta S_{\text{SnTi}}^{\text{f}} \) (J mol\(^{-1}\) K\(^{-1}\)) | 179808 |

* All parameters are given in J (mole of atoms)\(^{-1}\); Temperature (T) in K. The Gibbs energies for the pure elements are taken from the compilation of Dinsdale [16]. The underlined parameters have been evaluated in the current work. GHSEX (XX = NB, Sn and Ti) are the reference state of Gibbs energies.

- Liquid (\( \text{Nb,Sn,Ti} \))
  - \( L_{\text{Nb,Sn,Ti}}^{\text{f,liquid}} = \phi_{\text{Nb}} \cdot L_{\text{Nb}}^{\text{f,liquid}} + \phi_{\text{Sn}} \cdot L_{\text{Sn}}^{\text{f,liquid}} + \phi_{\text{Ti}} \cdot L_{\text{Ti}}^{\text{f,liquid}} \)

- Bcc (\( \text{Nb,Sn,Ti} \) \( \text{Va}_s \))
  - \( L_{\text{Nb,Sn,Ti}}^{\text{f,bcc}} = \phi_{\text{Nb}} \cdot L_{\text{Nb}}^{\text{f,bcc}} + \phi_{\text{Sn}} \cdot L_{\text{Sn}}^{\text{f,bcc}} + \phi_{\text{Ti}} \cdot L_{\text{Ti}}^{\text{f,bcc}} \)

- Hcp (\( \text{Nb,Sn,Ti} \) \( \text{Va}_h \))
  - \( L_{\text{Nb,Sn,Ti}}^{\text{f,hcp}} = \phi_{\text{Nb}} \cdot L_{\text{Nb}}^{\text{f,hcp}} + \phi_{\text{Sn}} \cdot L_{\text{Sn}}^{\text{f,hcp}} + \phi_{\text{Ti}} \cdot L_{\text{Ti}}^{\text{f,hcp}} \)

\[ \Delta F_{\text{TiSn}}^{\text{f}} = -141133 - 1.12727 + 3 \cdot \text{GHSERNB} + \text{GHSERSN} \]

\[ \Delta H_{\text{TiSn}}^{\text{f}} = 99547 + 3 \cdot \text{GHSERNB} + \text{GHSERSN} \]

\[ \Delta S_{\text{TiSn}}^{\text{f}} = 15000 + 3 \cdot \text{GHSERNB} \]

\[ \Delta G_{\text{NbSn}}^{\text{f}} = -66258.9 + 107 + 3 \cdot \text{GHSERNB} + \text{GHSERSN} \]

\[ \Delta H_{\text{NbSn}}^{\text{f}} = 106258.9 + 64.00867 + 3 \cdot \text{GHSERSN} + \text{GHSERNB} \]

\[ \Delta S_{\text{NbSn}}^{\text{f}} = 340853.17 + 24.4717 + 3 \cdot \text{GHSERSN} + \text{GHSERNB} \]

\[ \Delta G_{\text{NbTi}}^{\text{f}} = -23869.25 + 6 \cdot \text{GHSERT} + 3 \cdot \text{GHSERSN} \]

\[ \Delta H_{\text{NbTi}}^{\text{f}} = 48716.5 + 14.43437 + 3 \cdot \text{GHSERT} + 3 \cdot \text{GHSERSN} \]

\[ \Delta S_{\text{NbTi}}^{\text{f}} = 576942.9 + 15.7 \cdot \text{GHSERNB} + \text{GHSERT} \]

\[ \Delta G_{\text{SnSn}}^{\text{f}} = -50000 + 6 \cdot \text{GHSERNB} + 2 \cdot \text{GHSERSN} \]

\[ \Delta H_{\text{SnSn}}^{\text{f}} = -22403.9 + 3 \cdot \text{GHSERT} + 3 \cdot \text{GHSERSN} + 2 \cdot \text{GHSERNB} \]

\[ \Delta S_{\text{SnSn}}^{\text{f}} = -50000 + 6 \cdot \text{GHSERNB} + 2 \cdot \text{GHSERSN} \]

\[ \Delta G_{\text{SnTi}}^{\text{f}} = -25000 + 4 \cdot \text{GHSERT} + 2 \cdot \text{GHSERSN} \]

\[ \Delta H_{\text{SnTi}}^{\text{f}} = -117585.5 + 257 + 3 \cdot \text{GHSERT} + \text{GHSERNB} + \text{GHSERSN} \]

\[ \Delta S_{\text{SnTi}}^{\text{f}} = 20000 + 4 \cdot \text{GHSERT} + 3 \cdot \text{GHSERNB} + 3 \cdot \text{GHSERSN} \]

\[ \Delta G_{\text{SnTi}}^{\text{f}} = -50000 + 4 \cdot \text{GHSERNB} + \text{GHSERSN} \]

\[ \Delta H_{\text{SnTi}}^{\text{f}} = -117585.5 + 257 + 3 \cdot \text{GHSERT} + \text{GHSERNB} + \text{GHSERSN} \]

\[ \Delta S_{\text{SnTi}}^{\text{f}} = 20000 + 4 \cdot \text{GHSERT} + 3 \cdot \text{GHSERNB} + 3 \cdot \text{GHSERSN} \]

\[ \Delta G_{\text{SnTi}}^{\text{f}} = -50000 + 4 \cdot \text{GHSERNB} + \text{GHSERSN} \]
where $y'$ and $y''$ are the site fractions of element in the first and second sublattices. $G_m^\phi$ indicates the Gibbs energy of a hypothetical state where the first and second sublattices are completely filled by $i$ and $j$, respectively. The second term of equation (3) describes the energy contribution due to ideal mixing in each sublattice. $L_{\text{rec}}$ represents the reciprocal parameter.

Using Thermo-Calc packages [27], the model parameters were evaluated according to the uncertainty of the experimental data, and the model parameters were optimized through experiments and errors during the evaluation process, until most of the selected experimental information can be considered within the expected uncertainty range. Table 2 shows the thermodynamic parameters obtained in the current work.
4. Results and discussion

Figures 2 and 3 show the calculated isothermal sections of the Ti-Nb-Sn system at 700 and 900 °C compared with experimental information [10, 11], respectively. The chemical compositions of the annealed alloys together with the corresponding equilibrium phases are displayed in the figures. Due to small solid solubility or limited experimental verification, ternary solid solubility only considering the substitution between Ti and Nb was employed to describe intermetallic compounds, except Ti3Sn and Ti2Sn. The ternary solubilities of NbSn2, Ti5Sn3 and Ti2Sn3 phases were ignored due to the lack of experimental evidence. Table 3 shows the calculated solubilities of the third element in binary compounds compared with experimental data [10, 11]. As can be seen, the experimentally determined results can be well reproduced by the present calculations with the consideration of experiment errors.

3 three-phase regions at 700 °C and 4 three-phase regions at 900 °C have been experimentally verified by Wang et al [10, 11], signed by solid symbols in figures 2 and 3. As can be seen in figures 2 and 3, all the three-phase regions and most of the two-phase regions can be well reproduced based on the current thermodynamic modeling. A miscibility gap occurs in the bcc phase at 700 °C. As can be seen, the ternary solid solubility of bcc phase is large at Ti-rich region while small at Nb-rich region, almost no Sn solubility at the composition near 85 at.% Nb. This phenomenon may be caused by the over-stability of bcc phase at the Ti-Nb boundary near the Nb corner. Any attempt to enlarge the ternary solubility of the bcc phase near the Nb corner would cause unreasonable miscibility gap of bcc phase far away from the Ti-Nb boundary. As a result, the experimental data about several two-phase regions concerning the bcc phase have been given a small weight during the optimization process in order to achieve a general satisfaction. For the ternary compounds, Ti3Nb3Sn2 is stable at both 700 and 900 °C, while Ti3NbSn only stable at 900 °C. As can be seen, the thermal stabilities of Ti3Nb3Sn2 and Ti3NbSn can be well reproduced by using the current thermodynamic modeling, compared with the experimental information [10, 11].

Commonly, Ti based alloys undergo aging treatment after cooling in order to precipitate hcp α-Ti phase in bcc β-(Ti,Nb), which is an effective way to improve the mechanical properties. Consequently, it is interesting and technically important to know when the transformation from bcc β-(Ti,Nb) to hcp α-Ti takes place and how the alloying element influences the transformation. Figure 4 shows the influence of Nb and Sn content on the precipitation temperature and amount of hcp (α-Ti) phase in bcc β-(Ti,Nb) phase. According to the calculations, it is obvious that increasing the contents of Nb and Sn, especially Nb content, can significantly decrease the transformation temperature. Besides, when aging at 660 °C, the alloying of Nb and Sn may reduce the amount of hcp (α-Ti) precipitates. Thus, prior to experiment, the alloying composition and aging heat treatment schedule can be designed and optimized based on thermodynamic calculations to further obtain optimal properties.

| Compounds | Temperature, °C | Solubilities of the third element, at. % |
|-----------|----------------|----------------------------------------|
|           |                | Ti          | Nb          | Reference      |
| Ti3Sn     | 700            | 16.2        |             | [10]           |
|           | 900            | 14.1        |             | This work      |
| Ti5Sn     | 700            | over 13.9   |             | [10]           |
|           | 900            | 12.2        |             | This work      |
| Nb3Sn     | 700            | 21.3        |             | [10]           |
|           | 900            | 20.8        |             | This work      |
| Nb2Sn3    | 700            | over 19.3   |             | [11]           |
|           | 900            | 28.8        |             | This work      |
| Nb5Sn5    | 700            | no detection|             | [11]           |
|           | 900            | 44.4        |             | This work      |
| Nb3Sn     | 700            | over 7.4    |             | [11]           |
|           | 900            | 10.3        |             | This work      |

Table 3. Solubilities of the third element in binary compounds.
Figure 5 presents the Scheil solidification simulations of Ti-20Nb-xSn (x = 5, 10, 20 and 25) as-cast alloys. The Scheil solidification curves can provide various information like primary phase, transformation temperature, solidification path and so on. For a Ti-20Nb alloy, when the content of alloying element Sn is less than 20 wt.%, the primary phase would be bcc $\beta$-(Ti, Nb). While increasing Sn content to be 25 wt.%, the primary phase changes to be Ti$_3$NbSn. Moreover, large Sn content (over 20 wt.%) leads to the formation of Ti$_3$Sn. It can be seen that Scheil solidification simulations based on the current thermodynamic description of Ti-Nb-Sn system can predict the primary phase and solidification stage of as-cast alloys, which will affect the subsequent microstructure and performance of the alloy.

5. Conclusions

In this work, the phase equilibrium data of the Ti-Nb-Sn system has been evaluated. According to reliable experimental data, a thermodynamic description of the Ti-Nb-Sn system has been established. Comparisons between experimental and calculated isothermal sections at 700 and 900 °C show that most of the experimental data can be well accounted for by the current thermodynamic description. Based on thermodynamic calculations, the influence of the content of alloying elements Nb and Sn on the precipitation temperature and amount of hcp $\alpha$-Ti in
but are available from the corresponding author on reasonable request.

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Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

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