Thermo-Calc Software

TCS Nb-based Alloys Database (TCNB)

Examples Collection

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Contents

About the Database Examples

There are examples available to demonstrate both the *validity* of the database itself as well as to demonstrate some of its *calculation* capabilities when combined with Thermo-Calc software and its Add-on Modules and features.

For each database, the type and number of available examples varies. In some cases an example can belong to both a validation and calculation type.

- *Validation* examples generally include experimental data in the plot or diagram to show how close to the predicted data sets the Thermo-Calc calculations are. It uses the most recent version of the software and relevant database(s) unless otherwise specified.
- *Calculation* examples are intended to demonstrate a use case of the database. This might be showing a binary or ternary system calculated in a phase diagram, or demonstrate how the database and relevant software features would be applied to a heat treatment application, process metallurgy, soldering process, and so forth. In the case of heat treatment, it might include the result of calculating solidification segregation, determining homogenization temperature and then predicting the time needed to homogenize. There are many other examples specifically related to each database.

Where relevant, most references related to each example set are included at the end of the individual section. You can also find additional references specific to the database itself when using the database within Thermo-Calc. You can also contact us directly should you have any questions.

If you are interested in sharing your own examples using Thermo-Calc products in unique or surprising ways, or if you want to share your results from a peer reviewed paper, send an email to info@thermocalc.com.

TCS Nb-based Alloys Database (TCNB) Resources

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS Nb-based Alloys Database (TCNB) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, and the phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), and a list of the included elements.
- The *TCS Nb-based Alloys Database (TCNB) Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used.

Go to the Niobium-based Alloys page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCNB Validation Examples

In this section:

Predictions of Phase Equilibria

The TCS Nb-based Alloys Database (TCNB) can be used to calculate phase equilibria, including phase fractions and compositions, to reliably account for phase transformations. All the stable solution phases and intermetallic compounds that exist in the assessed and their extrapolated systems are included in the database. This version of the database (TCNB1) is able to predict the stable phases and phase compositions for a given composition and condition within the recommended composition range of the database.

The table shows the calculated phases and compositions in various Nb alloys compared with experimentally determined ones. The TCS Nb-based Alloys Database (TCNB)is able to predict the phase types at each given alloy composition and heat treatment temperature correctly and able to predict the phase compositions within the experimental errors.

Comparisons between the measured and the calculated (in parentheses) phase compositions						
Sample	***Phase***	***Nb (at.%)***	***Al (at.%)***	***Cr (at.%)***	***Ti (at.%)***	***Si (at.%)***
Nb-5Al-10Si-15Ti 1500 °C [1993Sub]	BCC	76 (77.7)	8 (6.0)		16 (14.6)	1 (1.7)
	Nb_5Si_3	49 (46.2)	3 (1.8)		14 (16.3)	34 (35.7)
Nb-5Al-24Ti-18Si 1500 °C [2006Zel]	BCC	62 (62.6)	7 (8.1)		29 (26.9)	0.5 (2.4)
	Nb_5Si_3	44 (42.8)	2 (1.8)		19 (19.7)	34 (37.5)
	M_3Si (4%)	(41.6)			(33.4)	(25.0)
Nb-10Cr-15Si-23Ti 1350 °C [2008Yan]	BCC	58.2 (60.3)		13.3 (13.9)	27.4 (24.3)	1.2 (1.5)
	Nb_5Si_3	42.2 (40.9)		0.6 (0.1)	21.2 (21.5)	36.1 (37.5)
	C_{14}	29.1 (23.0)		47.1 (54.2)	14.7 (11.9)	9 (10.9)
Nb-11Cr-13Si-23Ti 1350 °C [2008Yan]	BCC	59.4 (60.3)		13.5 (13.9)	26 (24.3)	1.2 (1.5)
	Nb_5Si_3	43.7 (40.9)		0.5 (0.1)	19.5 (21.5)	36.2 (37.5)
	C_{14}	26 (23.0)		51 (54.2)	13 (11.8)	10 (10.9)
Nb-9Al-14Si-18Ti 1450 °C [2020Sun]	Nb_5Si_3	49 (45.2)	4 (3.1)		15 (17.3)	32 (34.4)
	Nb_3Al*	67 (64.2)	13 (16.1)		15 (16.4)	5 (3.3)
	BCC	69 (68.3)	8 (11.0)		23 (19.3)	0 (1.4)
Nb-36Al-14Si-12Ti 1450 °C [2020Sun]	Nb_5Si_3	51 (45.2)	7 (5.9)		13 (17.3)	29 (31.6)

Comparisons between the measured and the calculated (in parentheses) phase compositions						
Sample	***Phase***	***Nb (at.%)***	***Al (at.%)***	***Cr (at.%)***	***Ti (at.%)***	***Si (at.%)***
	W_5Si_3	49 (50.6)	17 (22.4)		15 (11.9)	19 (15.1)
	AlTi_L10	28 (28.2)	55 (55.1)		17 (16.7)	0 (0.0)
	Al3Ti_D022	27 (23.8)	68 (72.5)		5 (3.7)	0 (0.0)
* Nb_3Al is modeled as Cr3Si_A15 in TCNB1						

References

[1993Sub] P. R. Subramanian, M. G. Mendiratta, D. M. Dimiduk, Microstructures and Mechanical Behavior of Nb-Ti Base Beta + Silicide Alloys. MRS Proc. 322, 491 (1993).

[2006Zel] K. Zelenitsas, P. Tsakiropoulos, Study of the role of Ta and Cr additions in the microstructure of Nb–Ti–Si–Al in situ composites. Intermetallics. 14, 639–659 (2006).

[2008Yan] Y. Yang, B. P. Bewlay, S. Chen, M. R. Jackson, Y. A. Chang, Effect of Cr Addition on the Multiphase Equilibria in the Nb-rich Nb-Si-Ti System - Thermodynamic Modeling and Designed Experiments. MRS Proc. 1128, 1128-U05-42 (2008).

[2020Sun] Z. Sun, W. Wu, X. Tian, F. Zhang, C. Ai, X. Zhang, Y. Li, X. Guo, Phase equilibria and multi-element interaction study in the metal-rich side of the Nb–Ti–Si–Al quaternary system. Intermetallics. 120, 106760 (2020).

Solidification: Phase Formation

You can also use the TCS Nb-based Alloys Database (TCNB) to study solidification and phase formation. A conventional Scheil simulation provides an upper boundary for how far a solidification can deviate from equilibrium, therefore a real solidification is expected to occur between the equilibrium simulation and the Scheil simulation. In Thermo-Calc performing a Scheil simulation always triggers an equilibrium simulation.

Read more about Scheil Solidification Simulations on our website, including how to select the right model for your simulation. If you are in Thermo-Calc, press F1 to search the help to learn about using Scheil.

The results in the table and figure below show that the phase types from Scheil simulations for the as-cast Nb-Si alloys are in consistent experimental observed ones.

Comparison between the phases observed from as-cast Nb-Hf-Si-Ti alloys [2007Yan] and those predicted from Scheil simulation

Alloy Composition	*Phases observed from as-cast alloys*	*Phases predicted from Scheil simulation*
Nb-7.5Hf-21Ti-16Si	Bcc, M3Si	Bcc, M3Si
Nb-12.5Hf-21Ti-16Si	Bcc, M3Si	Bcc, M3Si
Nb-10Hf-33Ti-16Si	Bcc, M3Si, M5Si3	Bcc, M3Si, M5Si3
Nb-8Hf-25Ti-22Si	Bcc, M3Si, Nb5Si3	Bcc, M3Si, Nb5Si3

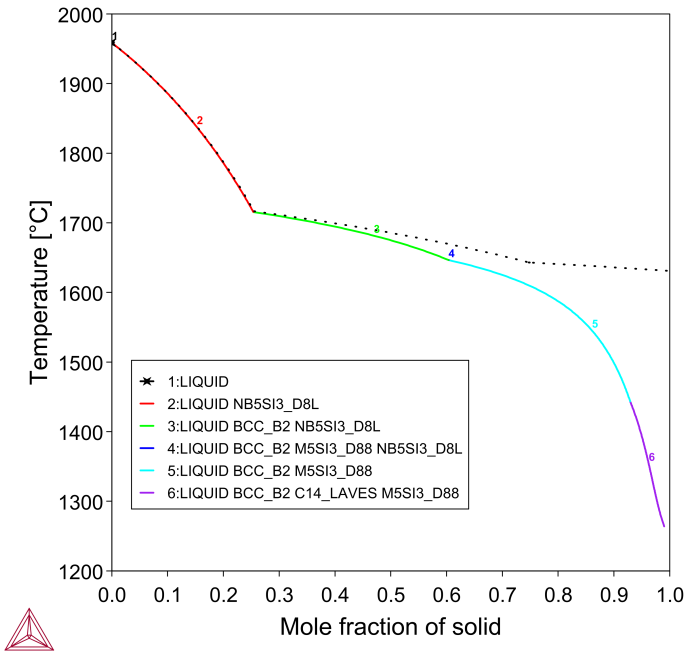

Figure 1: Calculated solidification path of Nb-5Al-5Cr-5Hf-2Mo-18Si-24Ti [2007Gen] using the Scheil and equilibrium model.

References

[2007Gen] 1. J. Geng, P. Tsakiropoulos, A study of the microstructures and oxidation of Nb–Si–Cr–Al–Mo in situ composites alloyed with Ti, Hf and Sn. Intermetallics. 15, 382–395 (2007).

[2007Yan] Y. Yang, B. P. Bewlay, Y. A. Chang, Liquid-Solid Phase Equilibria in Metal-Rich Nb-Ti-Hf-Si Alloys. J. Phase Equilibria Diffus. 28, 107–114 (2007).

TCNB Calculation Examples

In this section:

Binary Phase Diagrams

You can use the TCS Nb-based Alloys Database (TCNB) to plot binary phase diagrams in Thermo-Calc. Each assessed binary system is modeled to accurately describe experimental phase diagram data available in the literature. These examples show a selection of the important assessed systems that are the building blocks of the database itself when applying the CALPHAD method.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

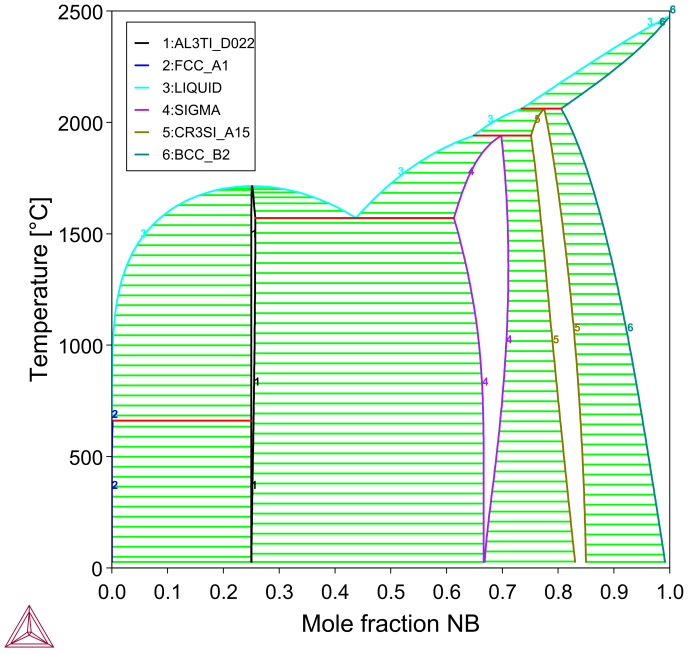

Figure 2: Calculated Al-Nb phase diagram.

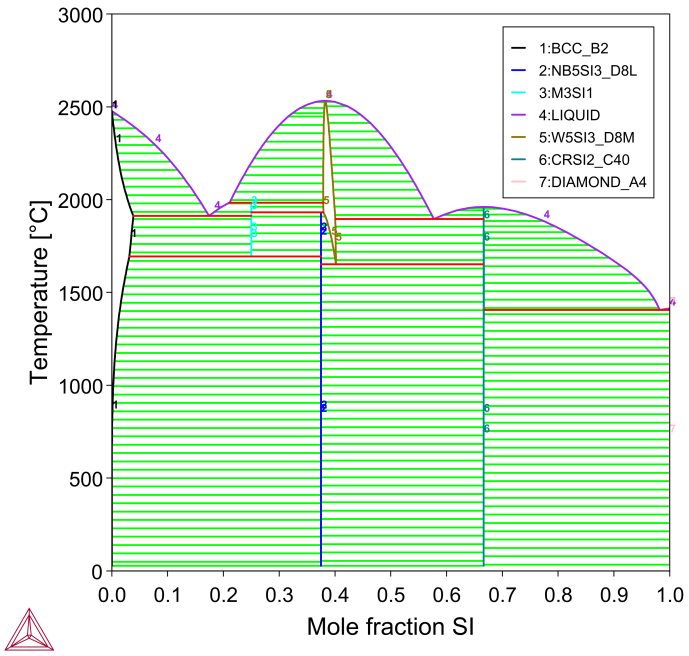

Figure 3: Calculated Nb-Si phase diagram.

Ternary Phase Diagrams

You can use the TCS Nb-based Alloys Database (TCNB) to plot ternary phase diagrams in Thermo-Calc. Each assessed ternary system is modeled to accurately describe experimental phase diagram data available in the literature. These examples show a selection of the important assessed systems that are the building blocks of the database itself when applying the CALPHAD method.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

When working in Thermo-Calc with ternary diagrams you use either the Ternary Calculator (in Graphical Mode) or the Ternary module (in Console Mode). The fundamental calculation engine is the same but you access the settings in different ways.

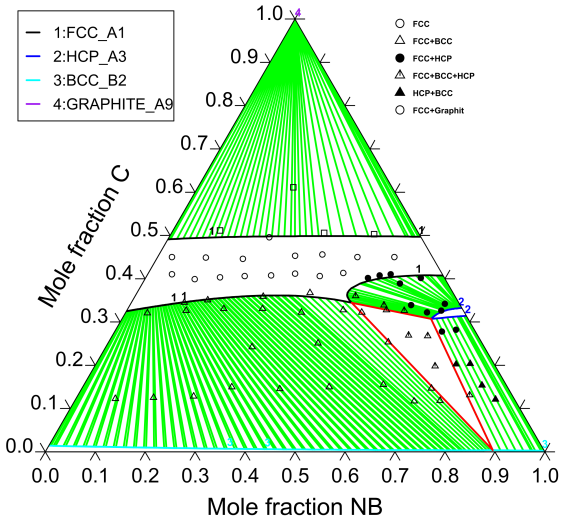

Figure 4: Calculated C-Nb-Ti isothermal section at 1773 K with experimental data from [1965Fed] and [1970Rud].

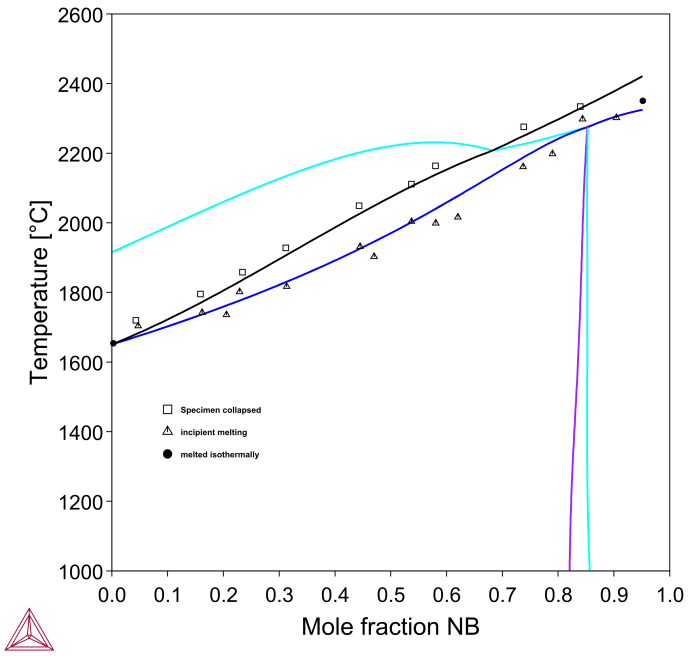

Figure 5: Calculated vertical section of C-Nb-Ti at 5 at. % C with experimental data from [1970Rud].

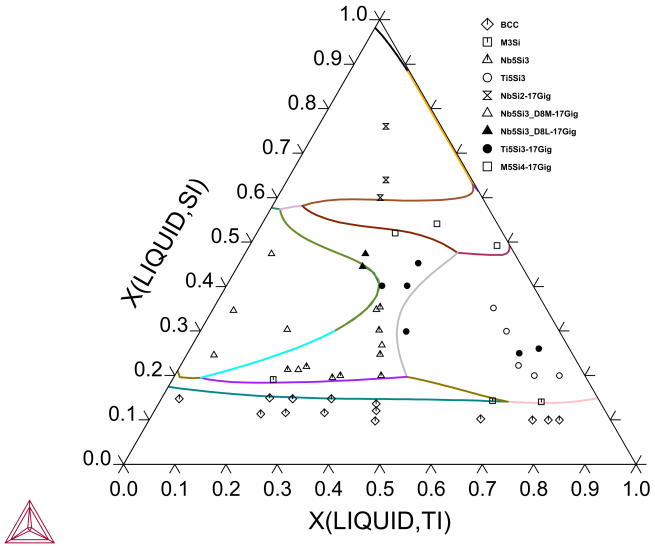

Figure 6: Calculated Nb-Si-Ti liquidus projection with experimental data from [1997Bew] and [2017Gig].

References

[1965Fed] T.F. Fedorov, N.M. Popova, E.I. Gladyshevskii, Ternary systems Hf-Nb-C, Zr-Nb-C, and Ti-Nb-C, Izv. Akad. Nauk. SSSR, Met. (1965) 158–163.

[1970Rud] E. Rudy, Phase Equilibrium Investigation of Binary, Ternary, and Higher Order Systems. I. Phase Diagrams of the Systems Titanium-Niobium-Carbon, Titanium-Tantalum-Carbon, and Titanium-Molybdenum-Carbon, Mater. Res. Lab., Aerojet- Gen. Corp., Sacramento, CA, USA, 1970.

[1997Bew] B. P. Bewlay, M. R. Jackson, H. A. Lipsitt, The Nb-Ti-Si ternary phase diagram: Evaluation of liquid- solid phase equilibria in Nb-and Ti-rich alloys. J. Phase Equilibria. 18, 264–278 (1997).

[2017Gig] J. C. Jânio Gigolotti, G. C. Coelho, C. A. Nunes, P. A. Suzuki, J.-M. Joubert, Experimental evaluation of the Nb Si Ti system from as-cast alloys. Intermetallics. 82, 76–92 (2017).