Thermo-Calc Software

TCS Ti/TiAl-based Alloys Database (TCTI)

Examples Collection

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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 Ti/TiAl-based Alloys Database (TCTI) 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 Ti/TiAl-based Alloys Database (TCTI) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, plus phases and models. It also includes details about the thermophysical properties data (e.g. viscosity, surface tension, etc.), the elastic properties (elastic moduli and constants), a list of the included elements, and summaries of the database revision history by version.
- The *TCS Ti/TiAl-based Alloys Database (TCTI) 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 Titanium and TiAl-based Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to titanium and TiAl including links to resources such as examples, publications, and more.

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

TCTI Validation Examples

Some diagrams are calculated with earlier versions of the database. Negligible differences might be observed if these are recalculated with the most recent version. The diagrams are updated when there are considerable or significant improvements.

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Predictions of Phase Equilibria

The TCS Ti/TiAl-based Alloys Database (TCTI) can be used to calculate phase equilibria, including phase fractions and compositions, to reliably account for phase transformations with light impurities (O, N, H, etc.) taken into account. Typical examples for titanium alloys are shown with the emphasis on validation against experimental observations in multicomponent commercial alloys.

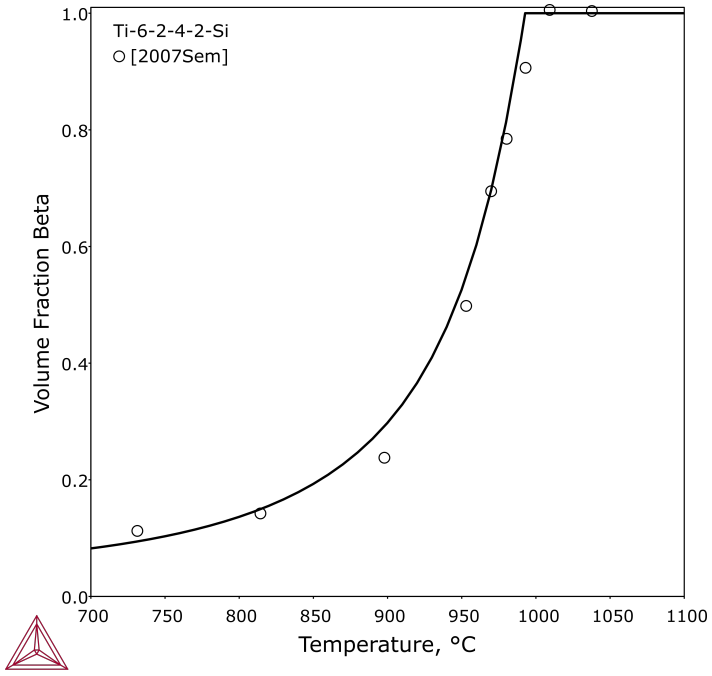

Figure 1: Calculated beta-approach curve for the Ti-6Al-2Sn-4Zr-2Mo-0.1Si alloy [2007Sem].

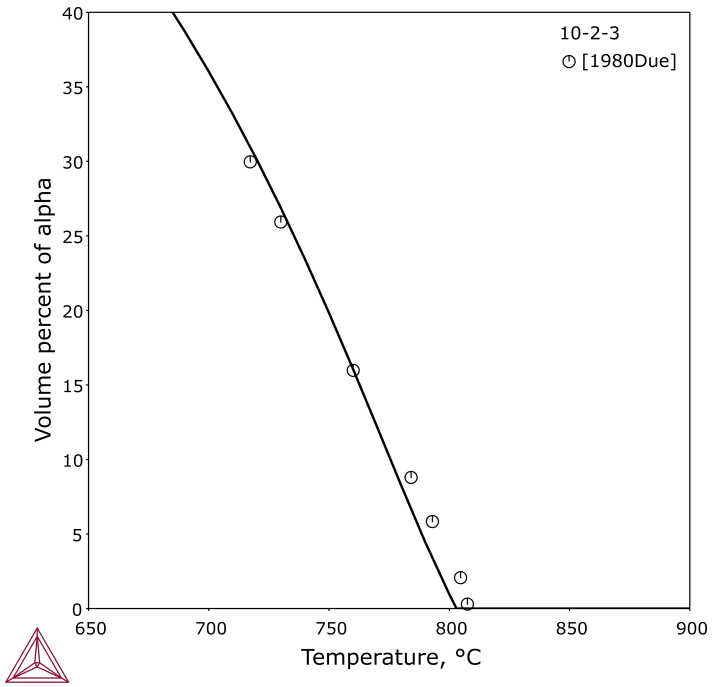

Figure 2: Calculated volume percent of alpha phase for the Ti-10-2-3 alloy [1980Due].

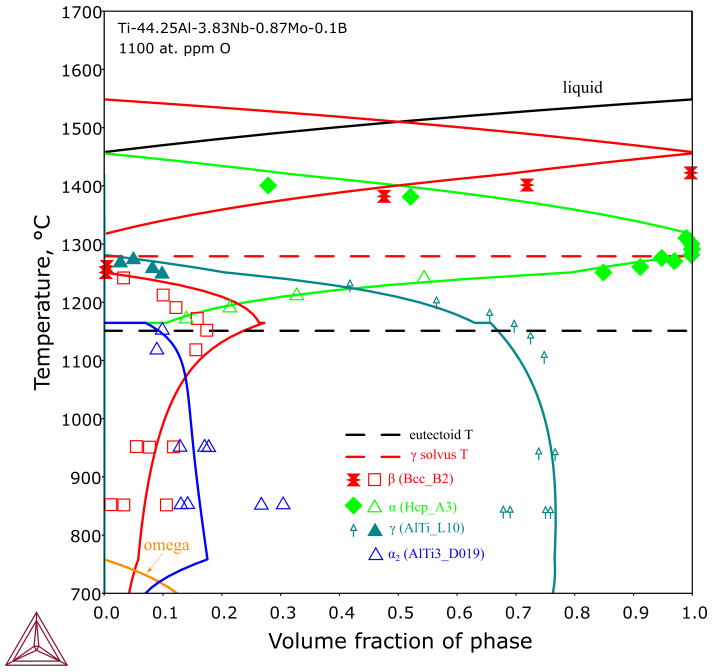

Figure 3: Calculated phase fraction vs. temperature for the Ti-44.25Al-3.83Nb-0.87Mo-0.1B alloy.

References

[1980Due] T. W. Duerig, G. T. Terlinde, J. C. Williams, Phase transformations and tensile properties of Ti-10V-2Fe-3Al. Metall. Trans. A. 11, 1987–1998 (1980).

[2007Sem] S. L. Semiatin, T. M. Lehner, J. D. Miller, R. D. Doherty, D. U. Furrer, Alpha/Beta Heat Treatment of a Titanium Alloy with a Nonuniform Microstructure. Metall. Mater. Trans. A. 38, 910–921 (2007).

Transition Temperatures

The TCS Ti/TiAl-based Alloys Database (TCTI) can be used to analyze α- and β-transus temperatures as shown in these examples.

α-transus Temperature

The α-transus temperature is an important parameter to develop processing techniques that are essential to improve mechanical properties of γ-TiAl-based alloys.

Validations have been focused on α-transus temperatures in the development of the thermodynamic database. One example shows a comparison between calculated and measured α-transus temperatures in typical multicomponent alloys.

The reported α-transus temperatures—measured either from thermal analysis or with synchrotron diffractions—can be affected by the deviation from equilibrium conditions.

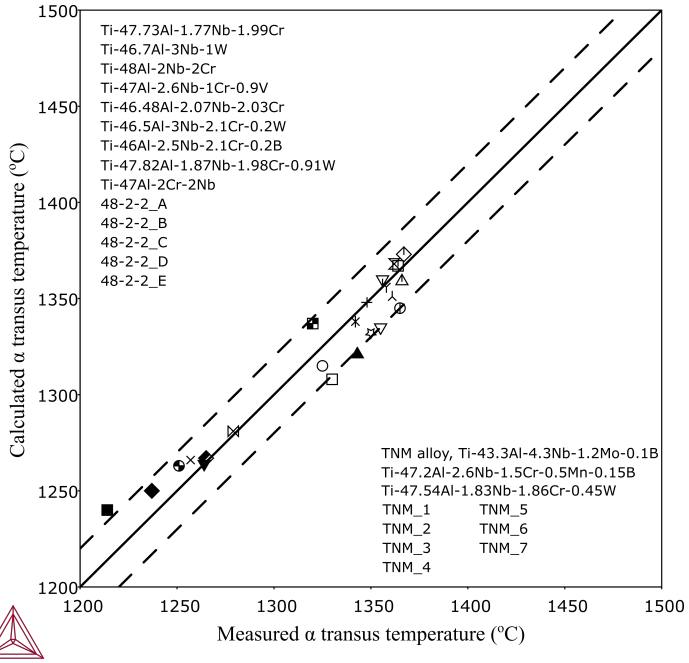

Figure 4: A comparison between measured and calculated α-transus temperatures compared to experimental data. The dash lines mark for ±20 °C deviations.

β-transus Temperature

Beta (β) transus temperature (T_β) is one of the important characteristics of titanium alloys. It is usually taken as the reference point to design a thermomechanical treatment. Therefore, knowledge of β-transus temperature is of critical importance to alloy design.

An important aspect for the development of the TCS Ti/TiAl-based Alloys Database (TCTI) is the validation of T_β for industrial alloys. With a well-determined composition for an alloy including impurities, it is feasible to predict T_β by performing a *single point equilibrium* type of calculation.

The following table is an example on the stable predictions of T_β from this thermodynamic database for variant Ti-64 investigated in references.

Ti-64 ***Composition (wt%, impurities in wt. ppm)***							***Reference***	***Tβ(exp.), °C***	***Tβ(calc.), °C***
Al	V	O	Fe	C	N	H			
6.1	4.1	2400	300	200	100	-	[1991Lee]	1005	994
6.04	4.03	900	1200	300	90	23	[1998Ahm]	994	989
6.4	4.2	1900	1400	160	50	40	[2003Sem]	1000	991
6	4.2	1100	1700	140	90	28	[2005Elm]	975	981
6.16	3.98	1900	1500	150	70	-	[2014Sab]	995	991
6.33	4.07	1600	1900	100	100	48	[2019Sem]	988	987

In practice, designed alloys typically have a nominal or target chemistry and an allowable tolerance range for each element. Determining the sensitivity of T_β can be achieved for all combinations of chemistry within the allowed range, thus establishing a range for T_β rather than a single value based on nominal composition. This example is for an IMI 230 alloy, which presents the variation of T_β over the normal composition range in the corresponding table.

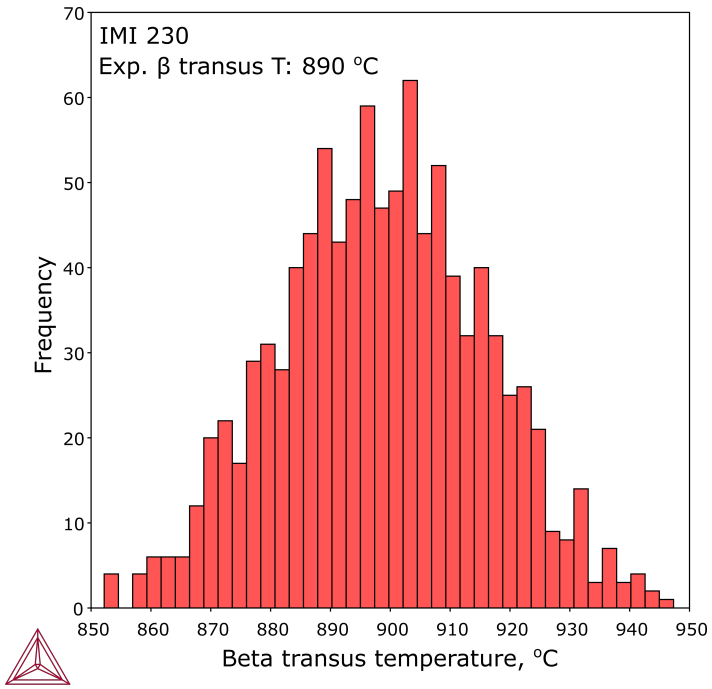

Figure 5: Variation in β-transus temperature over the normal composition range for IMI 230 alloy.

Element in IMI 230	*Minimum Wt%*	*Maximum Wt%*
Copper (Cu)	2.00	3.00
Iron (Fe)	-	0.20
Oxygen (O)	-	0.20
Carbon (C)	-	0.08
Nitrogen (N)	-	0.03
Hydrogen (H)		0.01

References

[1991Lee] Y. T. Lee, M. Peters, G. Welsch, Elastic moduli and tensile and physical properties of heat-treated and quenched powder metallurgical Ti-6Al-4V alloy. Metall. Trans. A. 22, 709–714 (1991).

[1998Ahm] T. Ahmed, H. J. Rack, Phase transformations during cooling in α+β titanium alloys. Mater. Sci. Eng. A. 243, 206–211 (1998).

[2003Sem] S. L. Semiatin, S. L. Knisley, P. N. Fagin, D. R. Barker, F. Zhang, Microstructure evolution during alpha-beta heat treatment of Ti-6Al-4V. Metall. Mater. Trans. A. 34, 2377–2386 (2003).

[2005Elm] J. W. Elmer, T. A. Palmer, S. S. Babu, E. D. Specht, In situ observations of lattice expansion and transformation rates of α and β phases in Ti–6Al–4V. Mater. Sci. Eng. A. 391, 104–113 (2005).

[2014Sab] M. Saby, E. Massoni, N. Bozzolo, A metallurgical approach to individually assess the rheology of alpha and beta phases of Ti–6Al–4V in the two-phase domain. Mater. Charact. 89, 88–92 (2014).

[2019Sem] S. L. Semiatin, M. Obstalecki, E. J. Payton, A. L. Pilchak, P. A. Shade, N. C. Levkulich, J. M. Shank, D. C. Pagan, F. Zhang, J. S. Tiley, Dissolution of the Alpha Phase in Ti-6Al-4V During Isothermal and Continuous Heat Treatment. Metall. Mater. Trans. A. 50, 2356–2370 (2019).

Molar Volume and Related Examples

The TCS Ti/TiAl-based Alloys Database (TCTI) contains all necessary volume data (including molar volume and thermal expansion) for most phases of importance to titanium alloys. This enables you to calculate properties related to molar volume, including volume fraction of phases, density, and thermal expansivity, as well as lattice parameters for cubic structures.

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

BCC Ti-Mo and Ti-V

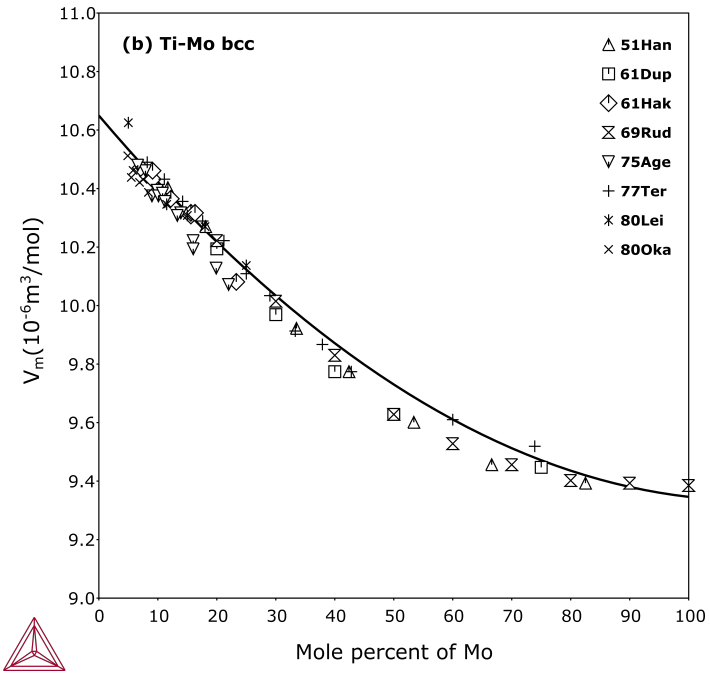

Figure 6: BCC molar volumes of Ti-Mo compared to experimental data.

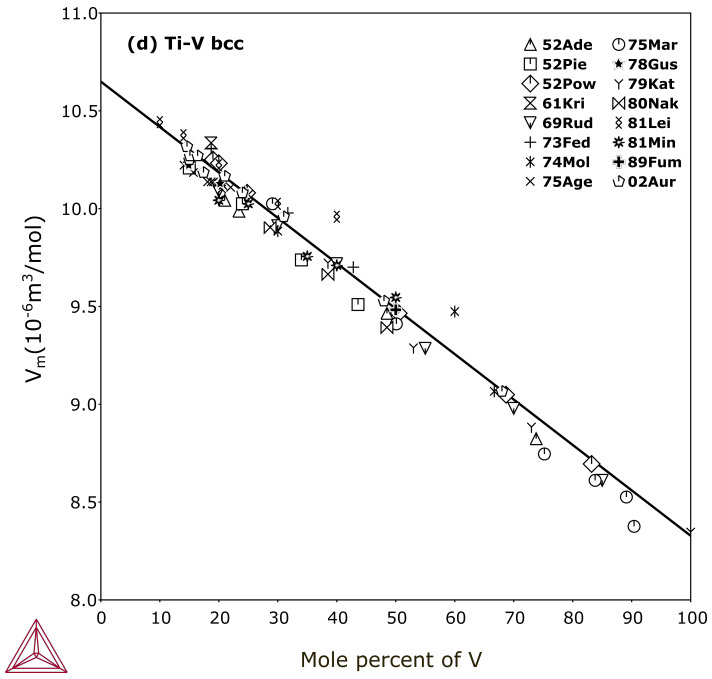

Figure 7: BCC molar volumes of Ti-V compared to experimental data.

HCP Ti-Al and Ti-Zr

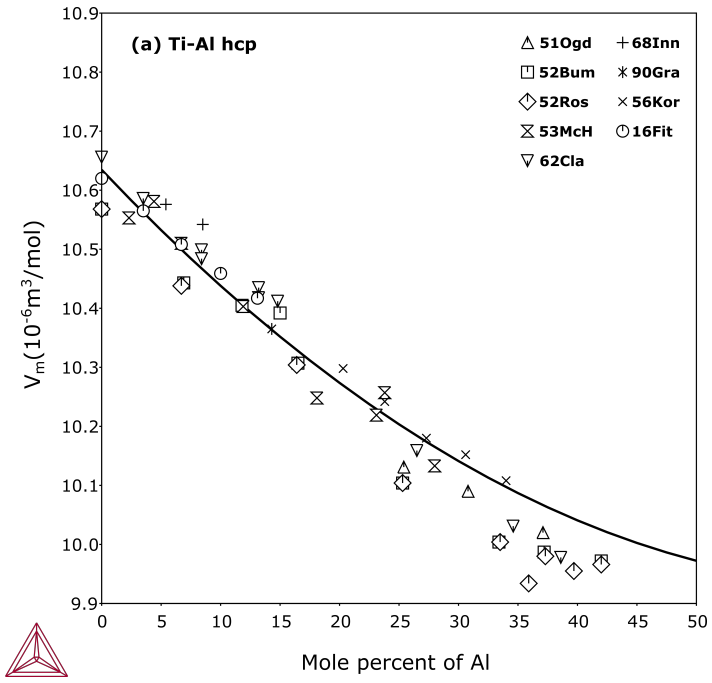

Figure 8: HCP molar volumes of Ti-Al compared to experimental data.

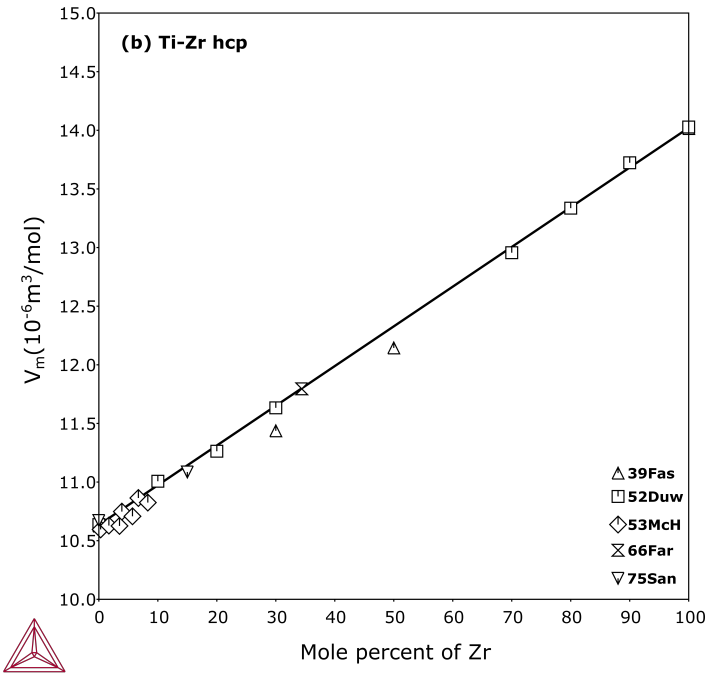

Figure 9: HCP molar volumes of Ti-Zr compared to experimental data.

Omega Ti-V and Ti-Nb

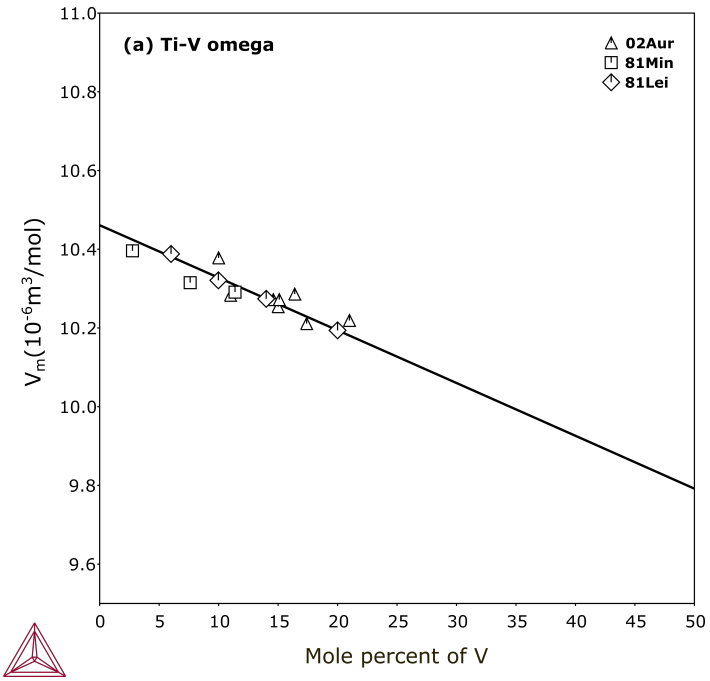

Figure 10: Omega molar volumes of Ti-V compared to experimental data.

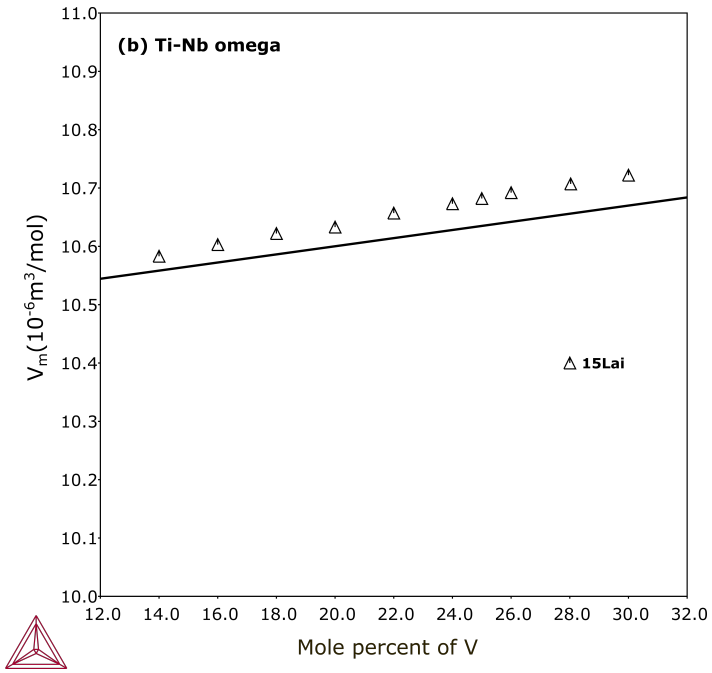

Figure 11: Omega molar volumes of Ti-Nb.

Linear Expansion and Density

Volume related properties, such as density and thermal expansion, are normally required as input for process simulations. A major achievement of the TCS Ti/TiAl-based Alloys Database (TCTI) is that such data can be readily calculated for different alloys from room temperature into the liquid state, which is of vital importance for process (e.g. casting, welding, etc.) simulations but difficult to measure or otherwise estimate.

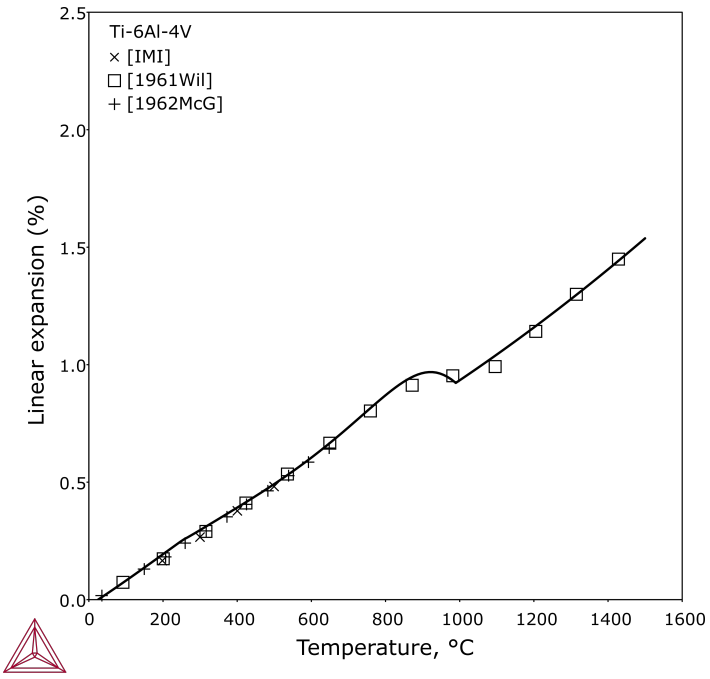

Figure 12: Linear expansion rate for Ti-6Al-4V. In this plot a good prediction can be made even in the region close to the β-transus where the amounts of α and β change rapidly with temperature..

Density is a fundamental material property. It is crucial for casting processes and to determine surface tension and viscosity from the measured raw data.

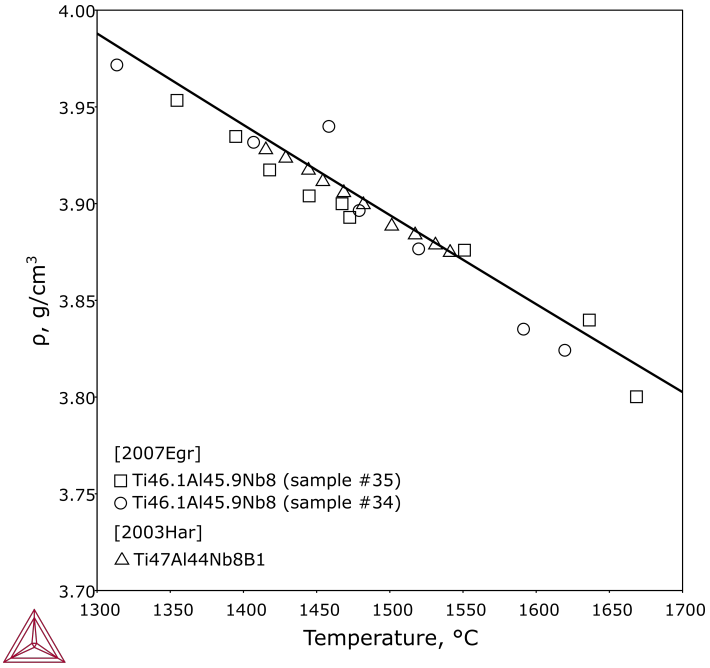

Figure 13: Density of liquid Ti-Al-Nb compared to experimental data.

The composition of Ti-45.5Al-8Nb is of high interest for investigations of TiAl-based alloys. This plot shows a comparison between calculated density and experimental data from room temperature to 1200 °C. With the assessed volume data in TCTI, it is possible to make accurate predictions on density covering a wide temperature range.

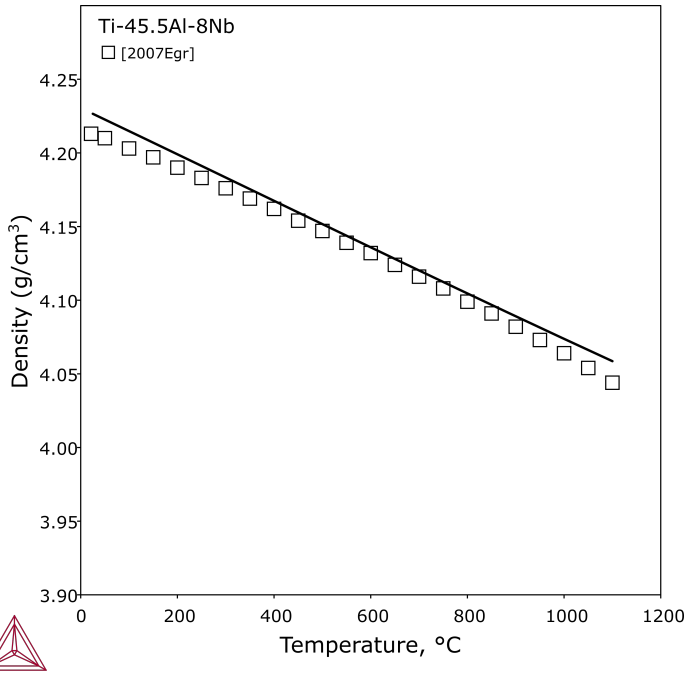

Figure 14: Calculated density of Ti-45.5Al-8Nb in a wide temperature range.

Applications to Process Simulations

The TCS Ti/TiAl-based Alloys Database (TCTI) database has thermophysical properties included. Below are examples about applications to process simulations.

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Enthalpy / Heat Contents

Process simulations are an important complement to experimental means in the optimization of casting and welding techniques. A key property for process simulations is enthalpy, which is needed to model the release of heat during the solidification process.

The example shows reliable predictions supported by experimental measurements using different techniques for enthalpy of Ti-64 in both solid and liquid states.

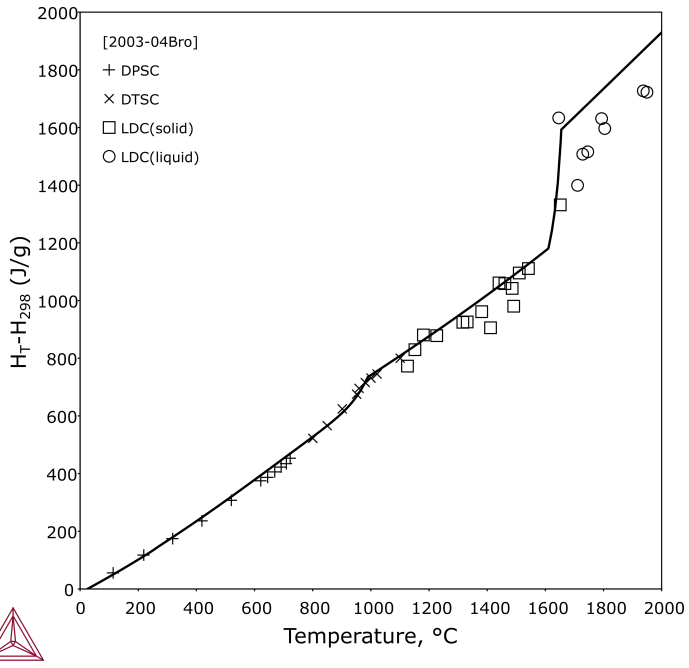

Figure 15: Enthalpy (H_T–H_{298}) of Ti-6Al-4V alloy [2003-04Bro].

Reference

[2003-04Bro] R. F. Brooks, J. A. J. Robinson, L. A. Chapman, M. J. Richardson, The enthalpy of a solid and liquid titanium-aluminum-vanadium alloy, High Temperatures-High Pressures, 35-36, 193-198 (2003-2004).

TCTI Surface Tension of Titanium Alloys

The TCS Ti/TiAl-based Alloys Database (TCTI) includes the surface tension thermophysical property data starting with version 3 (TCTI3).

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

The surface tension of the alloys $Ti_{48}Al_{48}Nb_2Cr_2$, $Ti_{46}Al_{46}Nb_8$, and $Ti_{46}Al_{46}Ta_8$ are measured with the oscillating drop technique in an electromagnetic levitation device under reduced gravity conditions on board a parabolic flight airplane. The measured values are compared with the experimental data from [2018Wun]. The deviations in these plots can be partially attributed to the challenges in measurements of these dynamic transport properties.

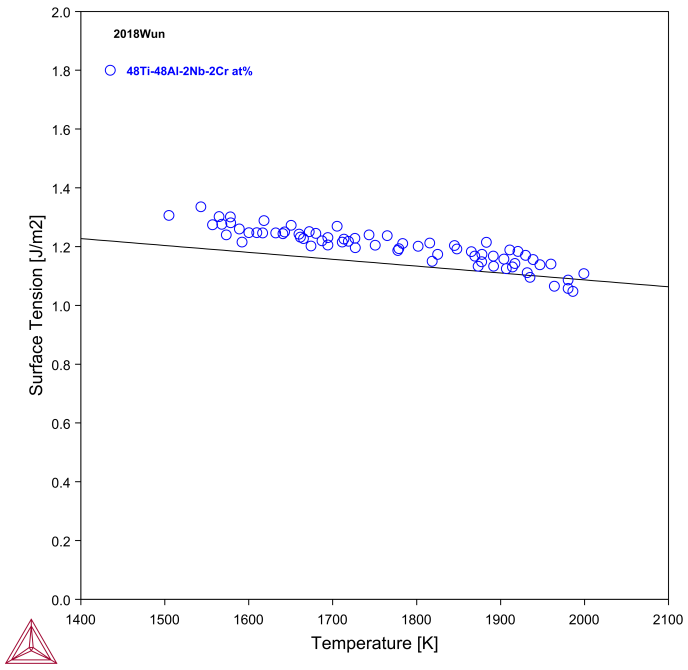

Figure 16: Surface tension of $Al_{48}Ti_{48}Nb_2Cr_2$. Experimental data are from [2018Wun].

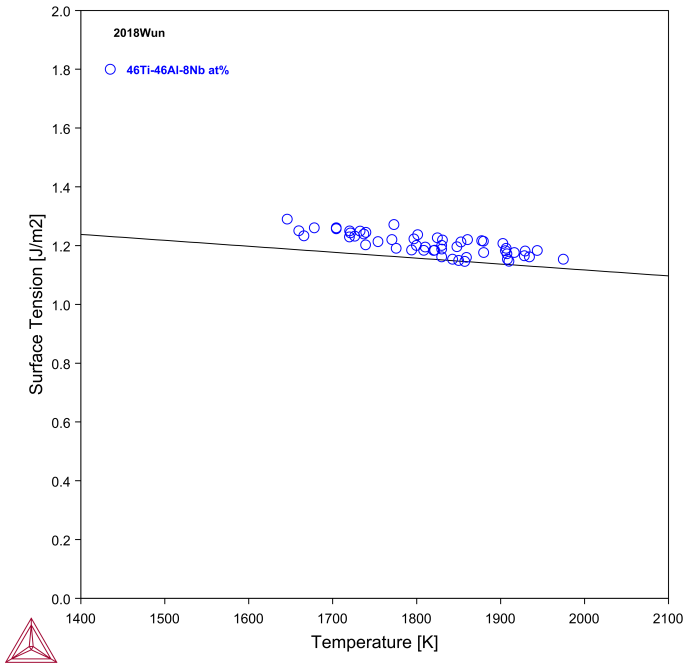

Figure 17: Surface tension of $Al_{46}Ti_{46}Nb_8$. Experimental data are from [2018Wun].

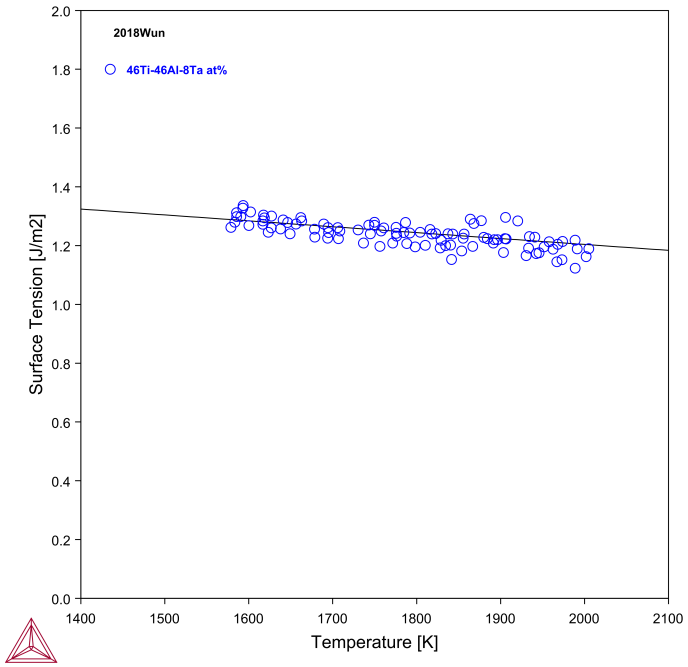

Figure 18: Surface tension of $Al_{46}Ti_{46}Ta_8$. Experimental data are from [2018Wun].

Ti64

The TCS Ti/TiAl-based Alloys Database (TCTI) predicts well-reproduced surface tension of Ti-6Al-4V, which is compared with different sets of experimental data.

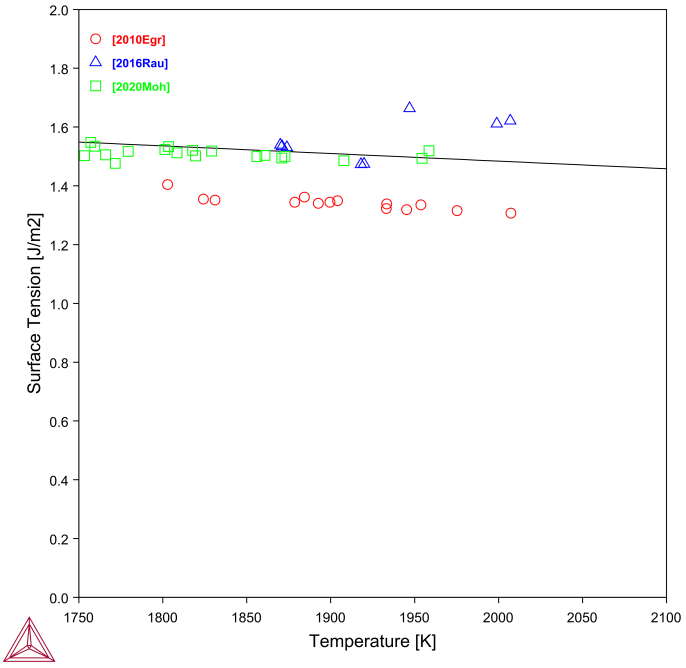

Figure 19: Surface tension of Ti-64. Experimental data are from [2010Egr; 2016Rau; 2020Moh].

References

[2010Egr] I. Egry, D. Holland-Moritz, R. Novakovic, E. Ricci, R. Wunderlich, N. Sobczak, Thermophysical Properties of Liquid AlTi-Based Alloys. Int. J. Thermophys. 31, 949–965 (2010).

[2016Rau] J. R. Raush, Ph.D. thesis, Thermophysical and Thermochemical Property Measurement and Prediction of Liquid Metal Titanium Alloys with Applications in Additive Manufacturing, Louisiana State University, Lafayette, LA, USA (2016).

[2020Moh] M. Mohr, R. Wunderlich, R. Novakovic, E. Ricci, H.-J. Fecht, Precise Measurements of Thermophysical Properties of Liquid Ti–6Al–4V (Ti64) Alloy On Board the International Space Station. Adv. Eng. Mater. 22, 2000169 (2020).

[2018Wun] R. K. Wunderlich, U. Hecht, F. Hediger, H.-J. Fecht, Surface Tension, Viscosity, and Selected Thermophysical Properties of Ti48Al48Nb2Cr2, Ti46Al46Nb8, and Ti46Al46Ta8 from Microgravity Experiments. Adv. Eng. Mater. 20, 1800346 (2018).

Electrical Resistivity of Some Commercial Ti Alloys

Using Thermo-Calc with the TCS Ti/TiAl-based Alloys Database (TCTI), you can calculate the quantities of a phase ϕ with the variable ELRS (ϕ) or a system (i.e. alloy) with ELRS. You can also calculate the derived quantity, i.e. electrical conductivity (ELCD) in a similar way.

The database includes electrical resistivity starting with version 4 (TCTI4).

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

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Ti-based Near-Alpha Alloy: Ti-6242Si

Ti-6Al-2Sn-4Zr-2Mo-0.08Si is usually categorized as a near-alpha alloy. You can make calculations for multicomponent titanium alloys with the modeled electrical resistivity.

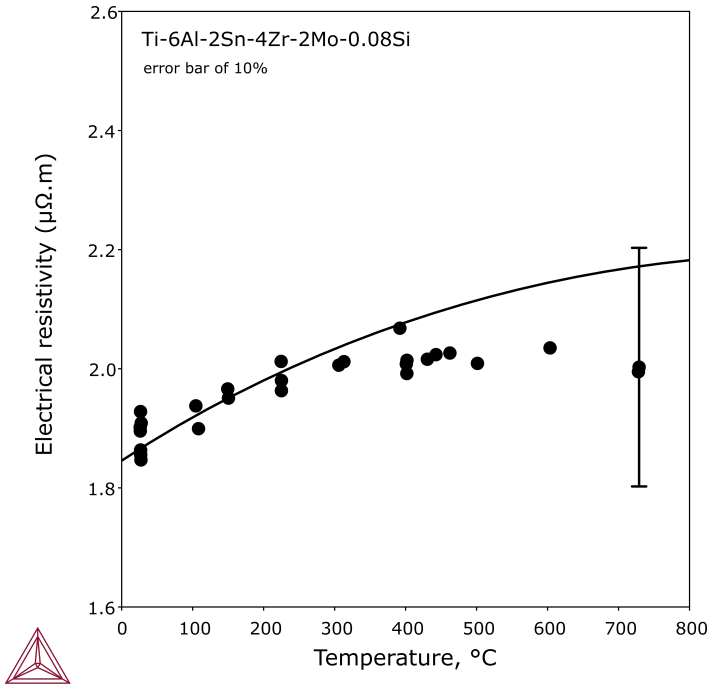

Figure 20: Calculated electrical resistivity of Ti-6242Si using the 'Equilibrium with Freeze-in Temperature' Property Model selected on the Property Model Calculator. The data are from [1994ASM].

Read more on our website about Property Models, including information about the Steel, Nickel, and Titanium Model Libraries, as well as how to create your own custom models in TC-Python. If you are in Thermo-Calc, press F1 to search the help.

Measured vs Calculated Electrical Resistivity

This example shows a comparison between measured and calculated electrical resistivity for a wide variety of commercial titanium alloys. The respective calculation is made by freezing-in the state at the typical heat treatment temperature of manufacture for each alloy. Deviations are expected, since electrical resistivity of alloys varies depending on the thermal-mechanical processing and actual composition. The black solid line in the plot indicates where calculated values are equal to experimental data. The blue dashed lines mark for 10% deviations while the pink dashed lines are for 15% deviations.

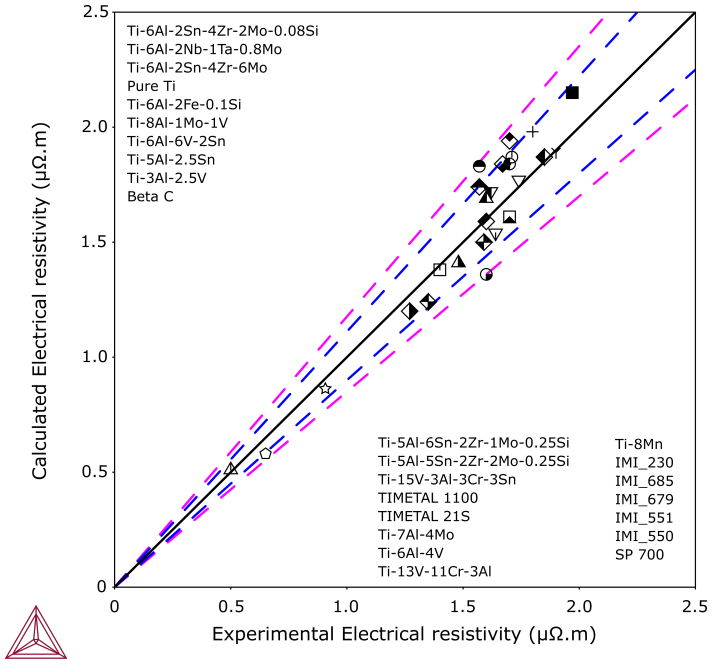

Figure 21: A comparison between measured and calculated electrical resistivity of various Ti-based alloys at room temperature. The data are from [1994ASM].

Reference

[1994ASM] R. Boyer, E. W. Collings, W. Gerhard (ed), Materials Properies Handbook: Titanium Alloys (ASM International, 1994).

Thermal Conductivity of Some Commercial Ti Alloys

Using Thermo-Calc with the TCS Ti/TiAl-based Alloys Database (TCTI), you can calculate the quantities of a phase ϕ with the variable THCD (ϕ), or a system (i.e. alloy) with THCD. You can also calculate the derived quantities, i.e. thermal resistivity (THRS) and thermal diffusivity (THDF), in a similar way.

The database includes thermal conductivity starting with version 4 (TCTI4).

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Ti-based Alpha-Beta Alloy: Ti-64

Ti-64 is the most well-known titanium alloy and is in widespread use. This example shows the calculated thermal conductivity of Ti-6Al-4V from 1300 to 2700 K. The plot shows that the data represented by blue squares are ~25% higher than the other two sets represented by cross and star symbols. Since it is a single β phase within this temperature range, scattering of experimental data can be attributed to the different measurement methods used in the experiments.

Read more on our website about Property Models, including information about the Steel, Nickel, and Titanium Model Libraries, as well as how to create your own custom models in TC-Python. If you are in Thermo-Calc, press F1 to search the help.

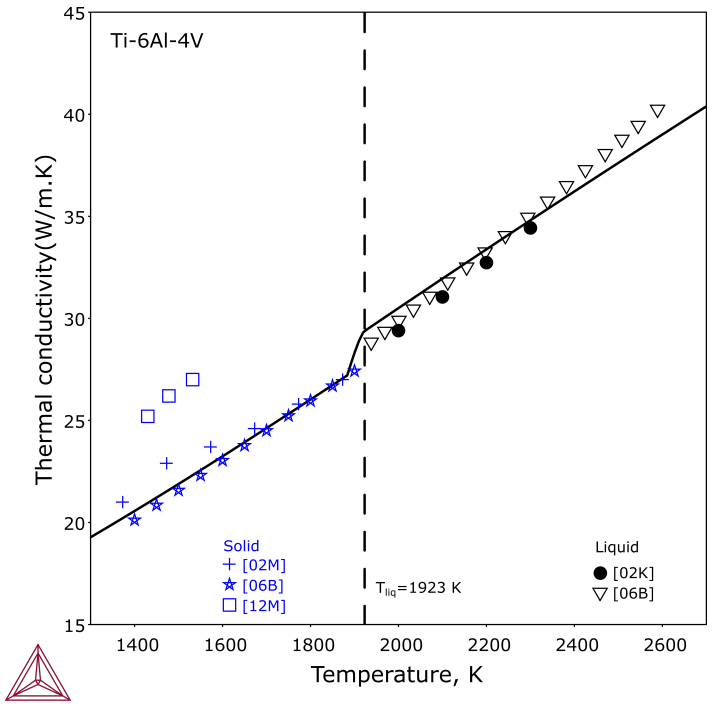

Figure 22: Calculated thermal conductivity of Ti-6Al-4V compared with experiment data. The dashed line indicates the liquidus temperature.

Measured vs Calculated Thermal Conductivity

This example shows a comparison between measured and calculated thermal conductivity for a wide variety of commercial titanium alloys. The respective calculation is made by freezing-in the state at the typical heat treatment temperature of manufacture for each alloy. Deviations are expected because the thermal conductivity of alloys varies depending on the thermal-mechanical processing and actual composition. The black solid line in the plot shows where calculated values are equal to experimental data. The blue dashed lines mark for 10% deviations while the red dashed lines are for 20% deviations.

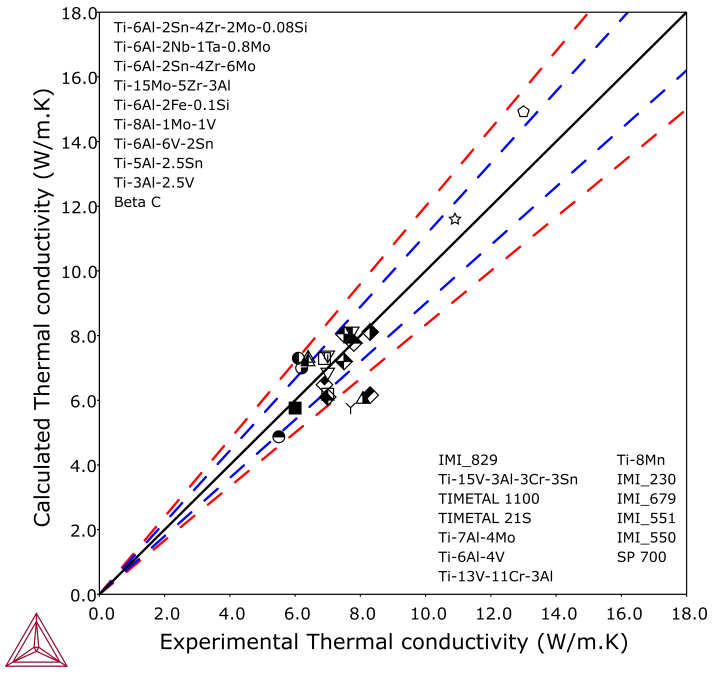

Figure 23: A comparison between measured and calculated thermal conductivity of various Ti-based alloys at room temperature. The data are from [1994ASM].

Reference

[1994ASM] R. Boyer, E. W. Collings, W. Gerhard (ed), Materials Properies Handbook: Titanium Alloys (ASM International, 1994).

Elastic Properties for FCC_A1, BCC_A2, and HCP_A3

The TCS Ti/TiAl-based Alloys Database (TCTI) (starting with version 6 (TCTI6) contains the necessary thermomechanical data for calculation of elastic constants and related elastic moduli for the three major phases FCC_A1, BCC_A2, and HCP_A3.

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

An example of the effect of oxygen concentration on Young's modulus in HCP_A3 titanium is included with the Thermo-Calc installation. The installed *T_19_Elastic_Properties_YoungsModulus_Ti-O.tcu* example is available from the **Thermo-Calc** Examples folder.

Pure Titanium

This example shows the temperature dependence of the independent elastic constants Cij of stable pure titanium. The color coding is black for C11, blue for C12, orange for C13, red for C33, and green for C44.

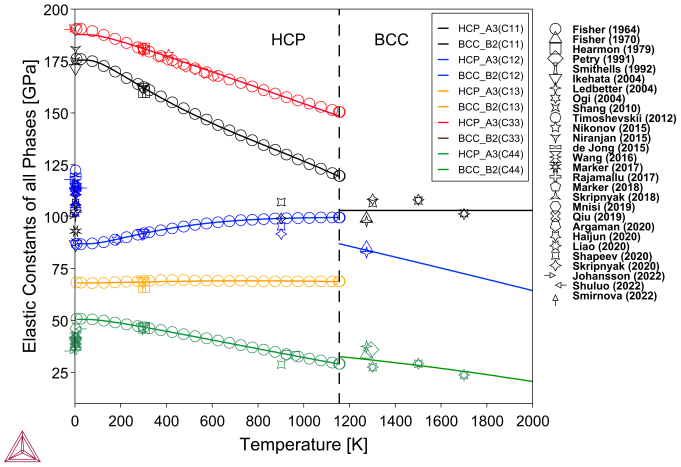

Figure 24: Independent elastic constants Cij of HCP_A3 and BCC_A2 titanium. Note, some data for BCC_A2 titanium is present below the transition temperature.

Literature vs Calculated Elastic Constants

This example shows a comparison between elastic constants taken from scientific literature, both experimental and theoretical, and calculated using our CALPHAD models for the TCTI unaries in different phases at different temperatures and a wide variety of titanium binaries and other important binary systems for titanium alloys in BCC phase at different temperatures and compositions. Metastable BCC titanium alloys are commonly sought after in biomedical applications for their bone tissue compatible mechanical properties.

The black line indicates perfect agreement between calculated and literature values. Some deviations are to be expected, since the derivation of elastic constants is not straight forward, and both typical *ab initio* calculations and experimental measurement methods have some inherent uncertainties. Therefore, deviations of a few percent, corresponding to several gigapascals, are normal. The color coding is black for C11, blue for C12, orange for C13, red for C33, and green for C44.

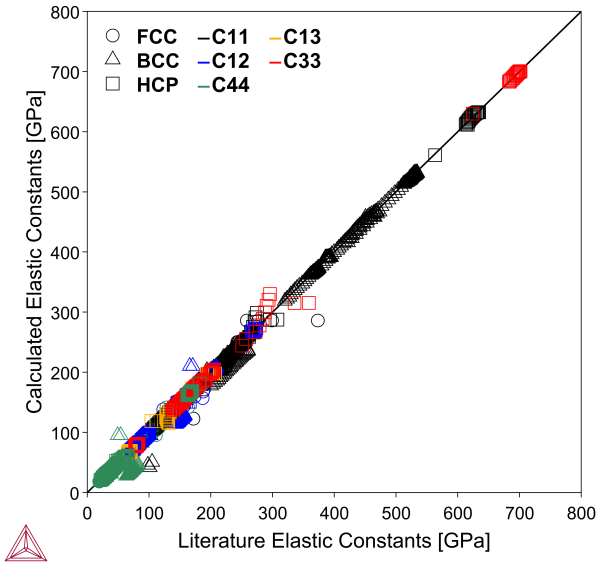

Figure 25: A comparison of literature and calculated elastic constants of TCTI unaries in different phases at different temperatures.

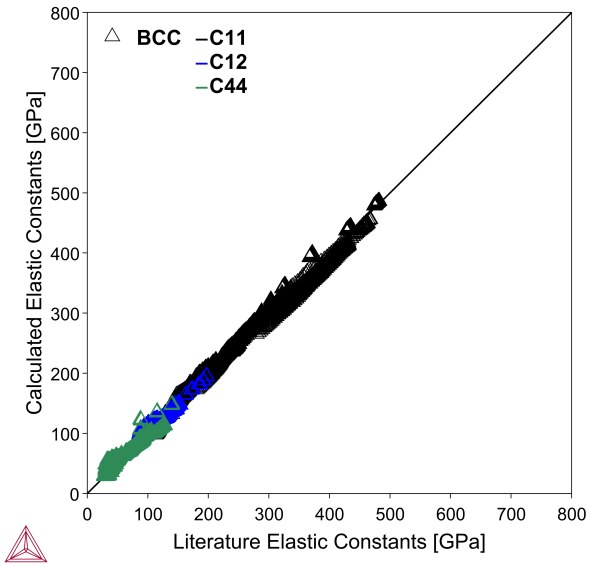

Figure 26: A comparison of literature and calculated elastic constants of TCTI titanium binaries and other important binary systems for titanium alloys in BCC phase at different temperatures and compositions.

BCC_A2 Ti-Ta Alloys

Titanium alloys are successful in the field of biomedical applications due to their mechanical properties and compatibility in biological environments. Compared to commercially pure titanium, metastable BCC titanium alloys can exhibit reduced elastic moduli, more closely matching that of human bone, reducing risk of stress shielding and bone resorption. There are a number of BCC stabilizers that allow titanium alloys to exist in the BCC phase at ambient conditions, one of which is tantalum.

This example shows the calculated elastic constants (Figure 27) and moduli (Figure 28) of metastable BCC_A2 Ti-Ta alloys. In both figures, the literature data and calculations are at 0 Kelvin, except for the black filled symbols and corresponding dashed line. Those represent Young's modulus values at room temperature (RT).

Only the elastic constants are assessed and then used to derive the elastic moduli, meaning the literature data in Figure 28 is standalone from the assessment work.

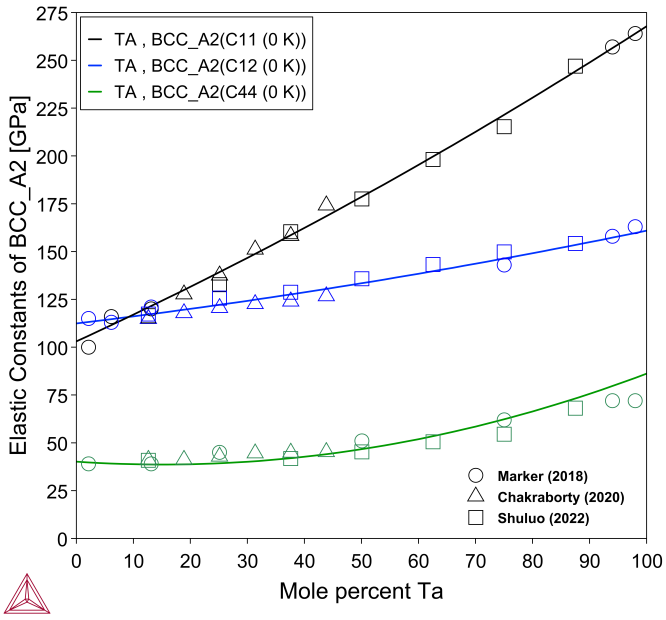

Figure 27: Calculated elastic constants at 0 K of metastable BCC_A2 Ti-Ta alloys. Open symbols represent DFT values from the literature.

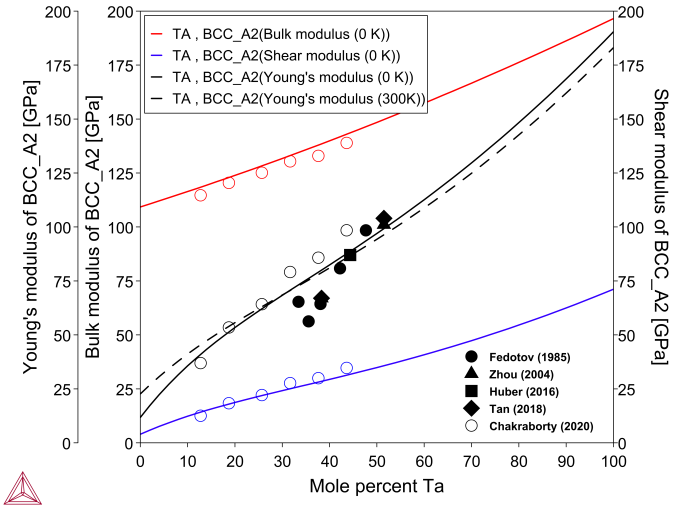

Figure 28: Calculated elastic moduli at 0 K, with the addition of Young's modulus measurements at RT of metastable BCC_A2 Ti-Ta alloys. Open symbols represent DFT values from the literature and filled symbols are from experiments. The dashed black line shows the calculated values of Young's modulus at RT.

TCTI Calculation Examples

Some diagrams are calculated with earlier versions of the database. Negligible differences might be observed if these are recalculated with the most recent version. The diagrams are updated when there are considerable or significant improvements.

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Ternary Systems 35
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Viscosity of Liquid for Ti-64 42
Electrical Resistivity and Conductivity of Titanium Alloys 43
Thermal Conductivity of Titanium Alloys 45
Applications Using the Diffusion Module (DICTRA) 47

Binary Systems

For the TCS Ti/TiAl-based Alloys Database (TCTI), each assessed binary system is modeled to accurately describe experimental phase diagram data available in the literature.

These examples are calculated binary phase diagrams, which can be created in Thermo-Calc using the BINARY module in Console Mode and the Binary Calculator in Graphical Mode.

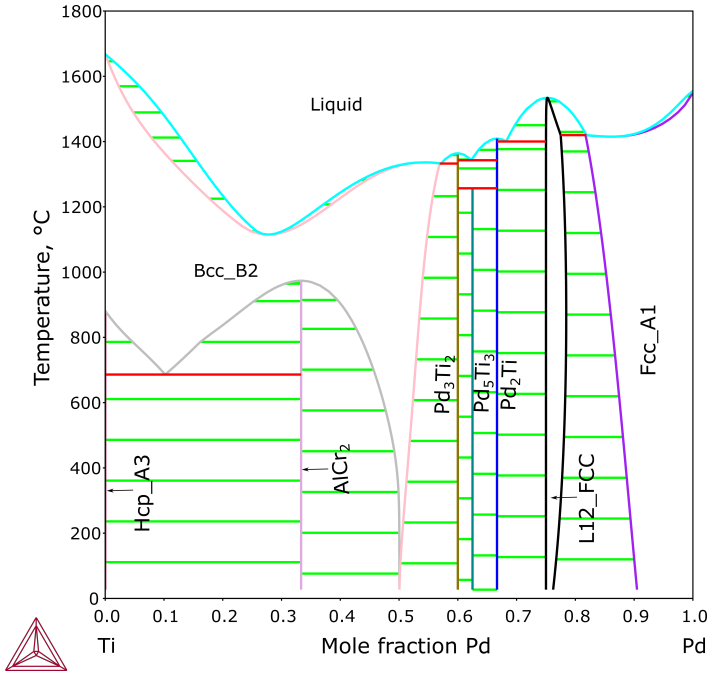

Figure 29: Calculated Ti-Pd phase diagram.

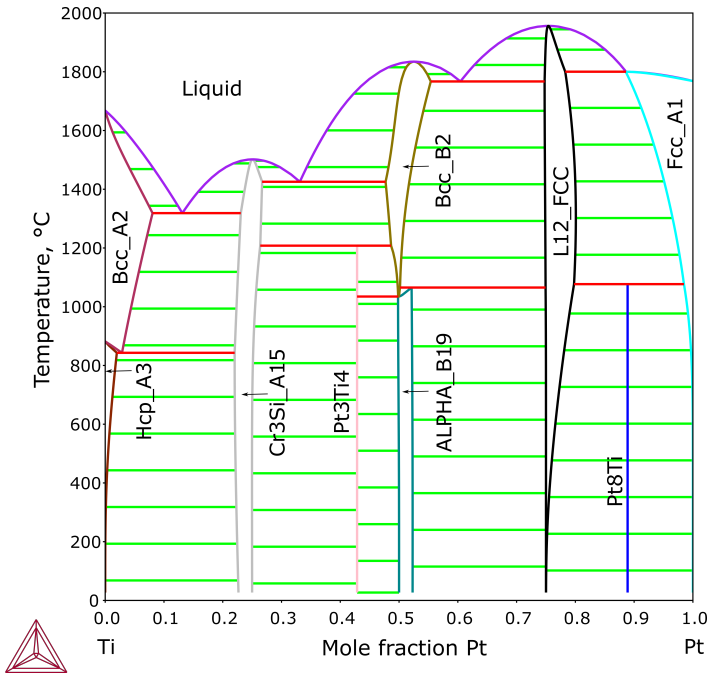

Figure 30: Calculated Ti-Pt phase diagram.

Ternary Systems

For the TCS Ti/TiAl-based Alloys Database (TCTI), these ternary system examples show the phase stabilities in two dimensional plots, isothermal or vertical sections. The ternary isothermal sections can be created in Thermo-Calc using the TERNARY module in Console Mode and the Ternary Calculator in Graphical Mode.

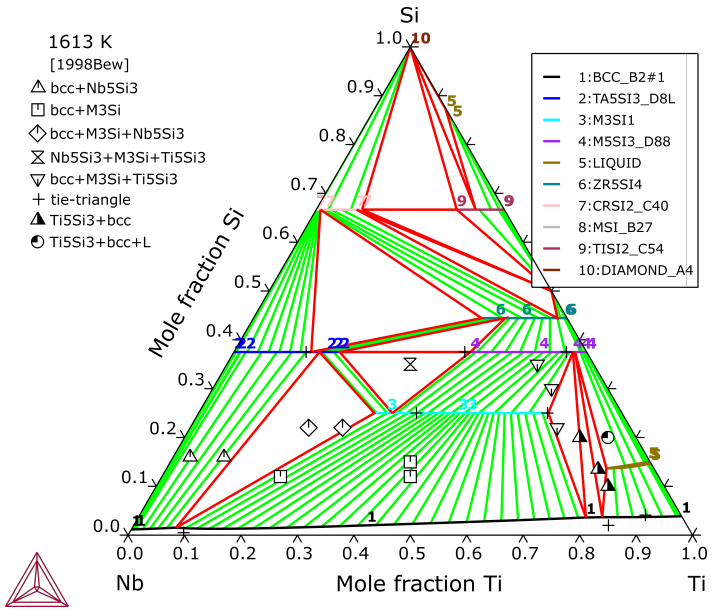

Figure 31: Calculated isothermal section of Ti-Nb-Si at 1613 K [1998Bew].

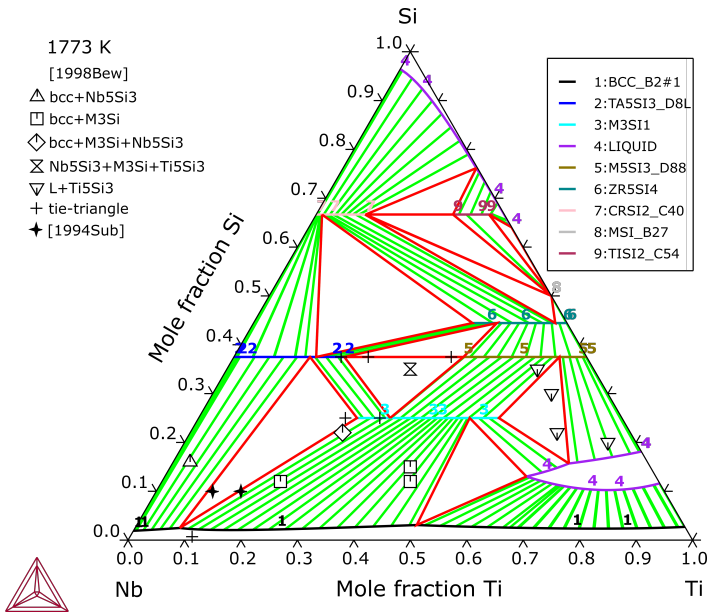

Figure 32: Calculated isothermal section of Ti-Nb-Si at 1773 K [1998Bew; 1994Sub].

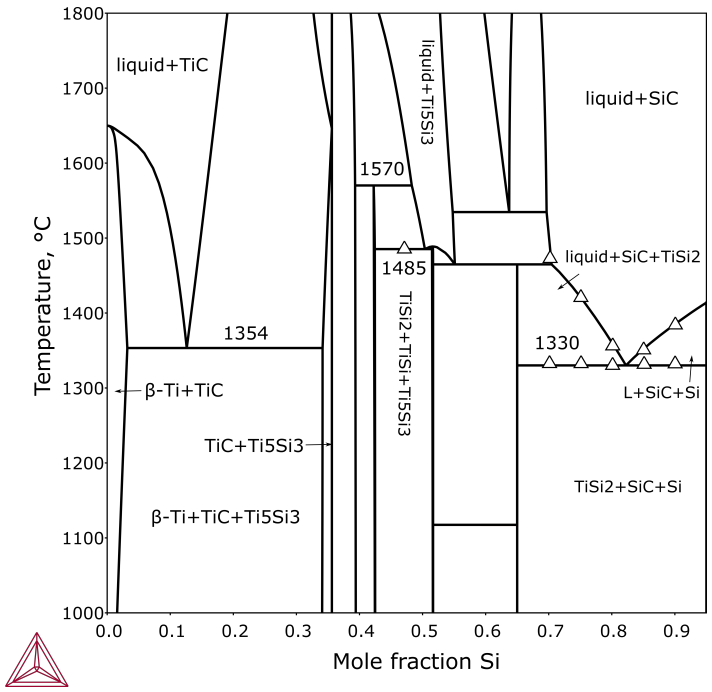

Figure 33: Calculated Ti-C-Si vertical section at 5 at%. Experimental data are from [2000Du].

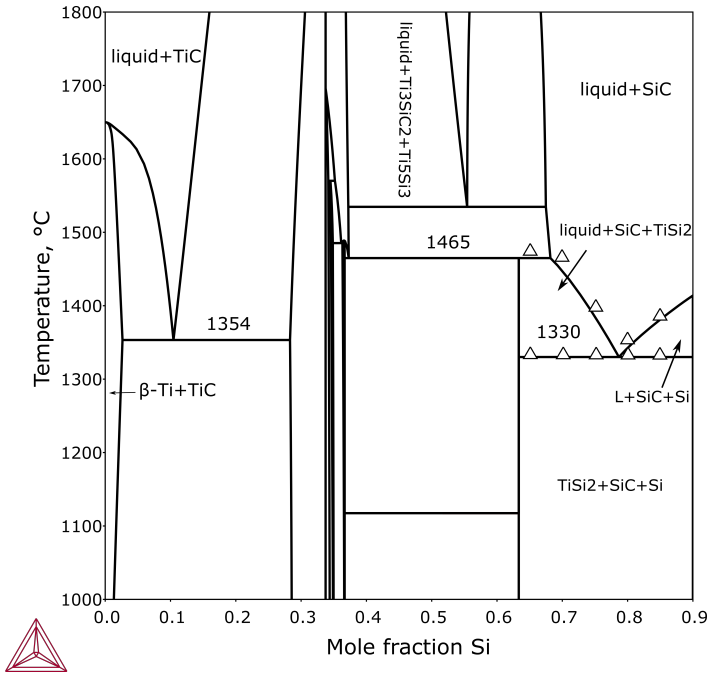

Figure 34: Calculated Ti-C-Si vertical section at 10 at% C. Experimental data are from [2000Du].

References

[1994Sub] P. R. Subramanian, M. G. Mendiratta, D. M. Dimiduk, in High Temperature Silicides and Refractory Alloys, Eds. C. L. Briant, J. J. Petrovic, B. P. Bewlay, H. A. Lipsitt, A. K. Vasudevan, Mater. Res. Soc. Symp. Proc. 322, Pittsburgh, PA, 491-502 (1994).

[1998Bew] B. P. Bewlay, M. R. Jackson, R. R. Bishop, The Nb-Ti-Si ternary phase diagram: Determination of solid-state phase equilibria in Nb- and Ti-rich alloys. J. Phase Equilibria. 19, 577–586 (1998).

[2000Du] Y. Du, J. C. Schuster, H. J. Seifert, F. Aldinger, Experimental Investigation and Thermodynamic Calculation of the Titanium-Silicon-Carbon System. J. Am. Ceram. Soc. 83, 197–203 (2000).

Impurity Elements

The impurity level in titanium alloys inevitably accounts for varying features such as β-transus temperature and phase fractions vs. temperature.

It is known that low amounts of interstitial impurities (such as O, C, and N) affect phase equilibria and transformations in both Ti- and TiAl-based alloys. Attributing to the high susceptibility to contamination of titanium alloys, it is suggested to rationally consider the effects from impurities for simulations.

This plot shows with increasing amount of oxygen, both Hcp_A3 and AlTi3_D019 phases get stabilized.

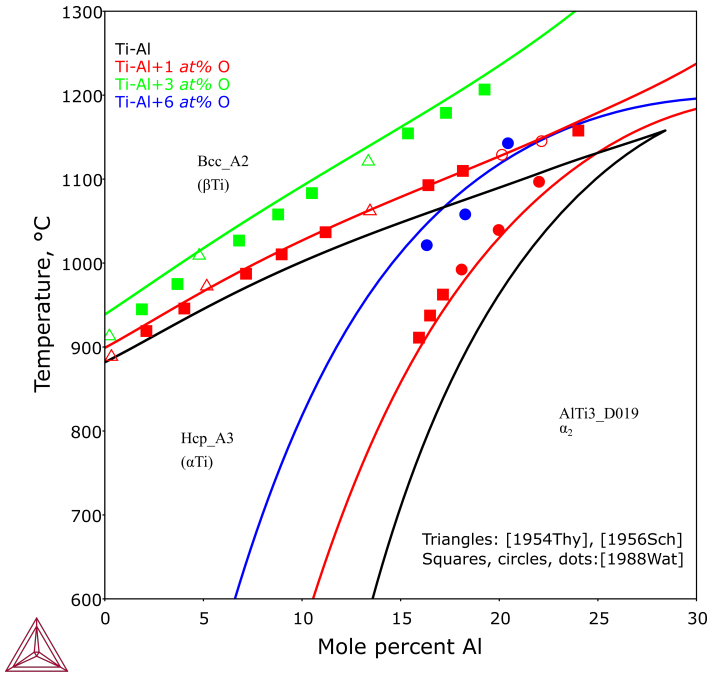

Figure 35: Influence of oxygen on the phase boundaries in the Ti-Al system.

Hydrogen is also incorporated in the thermodynamic TCS Ti/TiAl-based Alloys Database (TCTI), where hydrogen solubilities in solutions and stabilities of metal hydrides have been assessed.

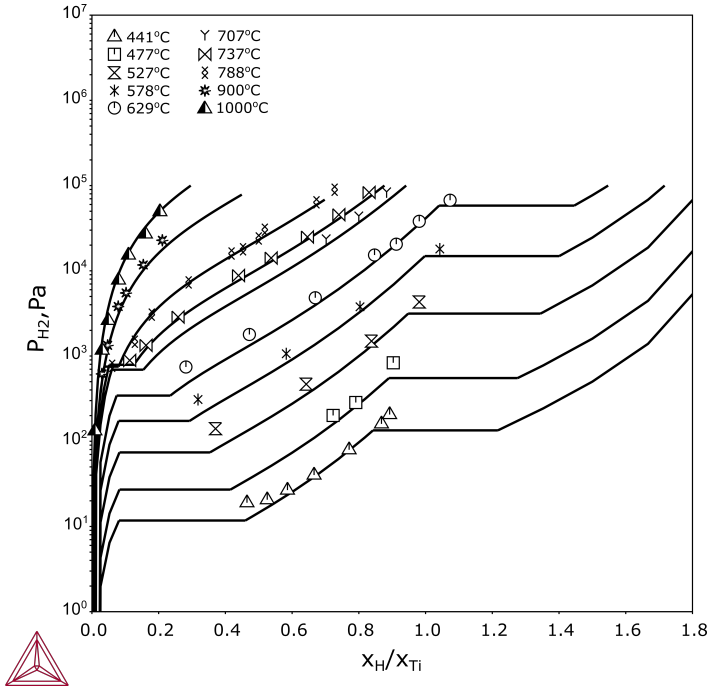

Figure 36: Calculated pressure-composition isotherms of the Ti-H system compared with experimental data cited in [1987San].

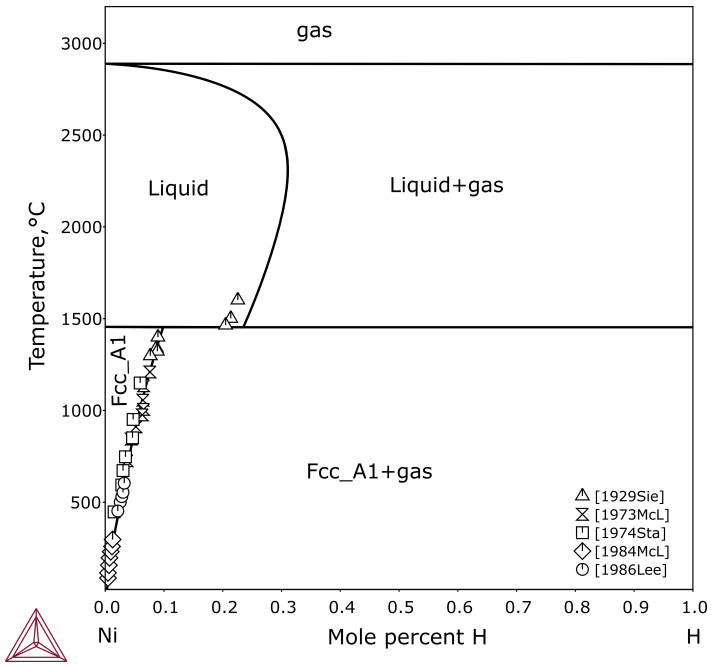

Figure 37: Calculated Ni-H phase diagram with experimental data from [1929Sie; 1973McL; 1974Sta; 1984McL; 1986Lee].

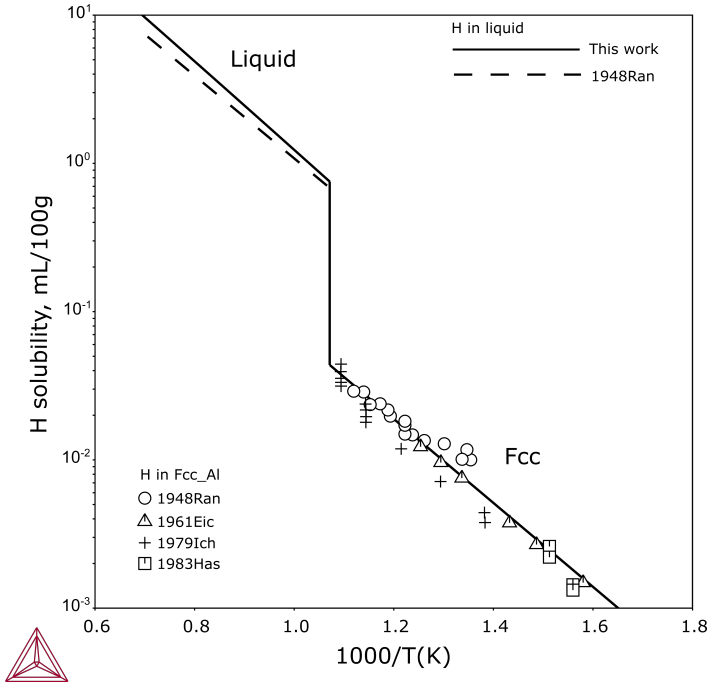

Figure 38: Calculated solubility of H in Al compared with experimental information from [1948Ran; 1961Eic; 1979Ich; 1983Has].

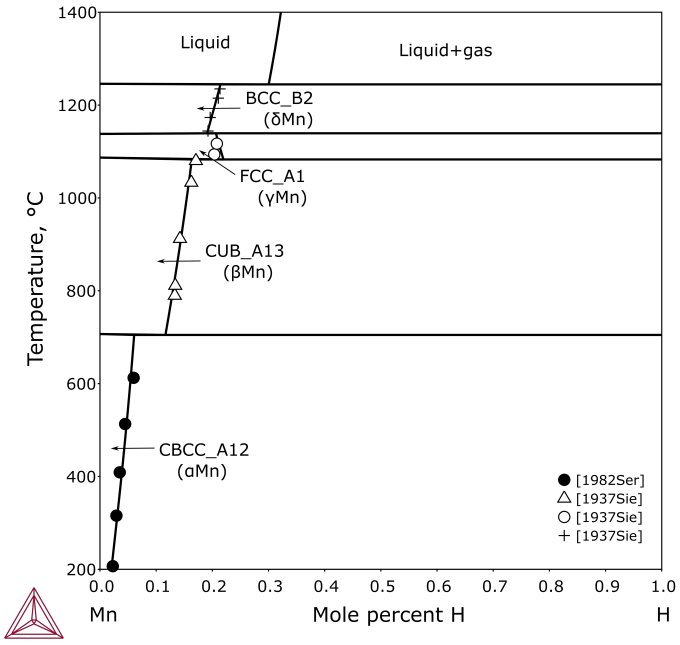

Figure 39: Calculated solubility of H in solid Mn compared with experimental data [1937Sie; 1982Ser].

References

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[1961Eic] V. W. Eichenauer, K. Hattenbach, A. Pebler, The solubility of hydrogen in solid and liquid aluminum. Zeitschrift für Met. 52, 682–684 (1961).

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[1986Lee] S.-M. Lee, J.-Y. Lee, The trapping and transport phenomena of hydrogen in nickel, Metall. Trans. A 17, 181–187 (1986).

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[1988Wat] R. M. Waterstrat, “Effect of Interstitial Elements on Phase Relationships in the Titanium-Aluminum System (NISTIR 88-3856)” (U.S. Dept. of Commerce, Arlington, Virginia, 1988).

Viscosity of Liquid for Ti-64

The TCS Ti/TiAl-based Alloys Database (TCTI) has viscosity thermophysical property data included starting with version 3 (TCTI3). Below are examples about applications to viscosity.

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

This plot shows the calculated viscosity of Ti-64 from assessed parameters compared with experimental data. The probable solid nucleation below the melting point in measurements could be one explanation for the shown deviations.

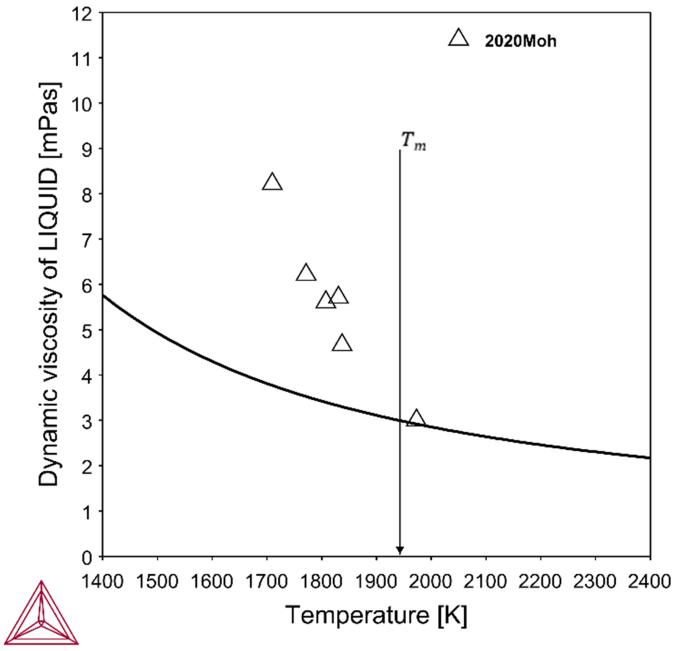

Figure 40: Calculated viscosity of liquid Ti-64 along with experimental data from [2020Moh].

Reference

[2020Moh] M. Mohr, R. Wunderlich, R. Novakovic, E. Ricci, H.-J. Fecht, Precise Measurements of Thermophysical Properties of Liquid Ti–6Al–4V (Ti64) Alloy On Board the International Space Station. Adv. Eng. Mater. 22, 2000169 (2020).

Electrical Resistivity and Conductivity of Titanium Alloys

A better understanding of electronic properties of alloys is beneficial to investigate alloying behavior and effects in solid solutions, as well as to facilitate studies on mechanical properties of titanium alloys.

Using Thermo-Calc with the TCS Ti/TiAl-based Alloys Database (TCTI), you can calculate the quantities of a phase ϕ with the variable ELRS (ϕ) or a system (i.e. alloy) with ELRS. You can also calculate the derived quantity, i.e. electrical conductivity (ELCD) in a similar way.

The database includes electrical resistivity starting with version 4 (TCTI4).

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Electrical Resistivity for Some Ti-based Alloys

In this example, the electrical resistivities for various alloys at room temperature are plotted as a function of alloy composition. The plot shows that the transition elements which lie close to titanium in the periodic table (i.e. Zr, Nb) bring about a relatively small increase in the resistivity of α-titanium, while the non-transition elements, whether substitutional or interstitial, appear to have a much greater effect.

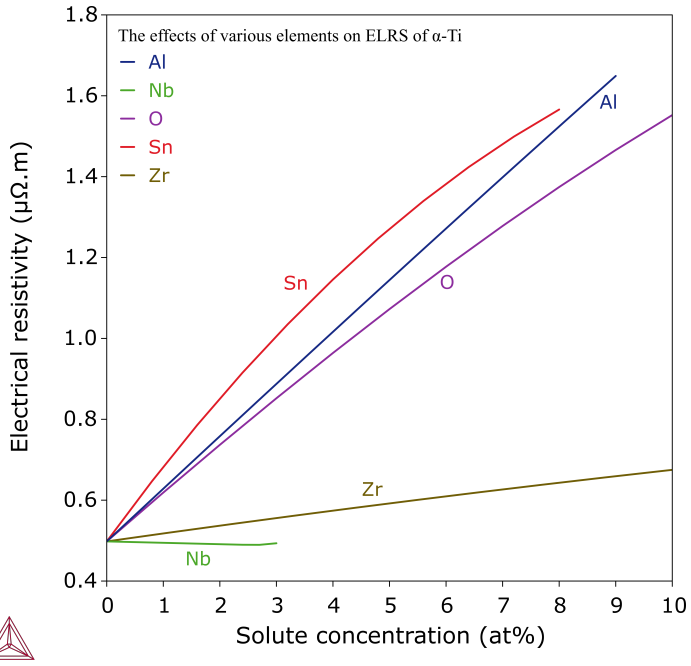

Figure 41: A comparison of the specific solute resistivities (dρ/dc) of Ti-based alloys.

Electrical Conductivity of Ti Metal and Ti Hydrides

In addition to electrical resistivity, you can also make calculations for electrical conductivity (ELCD) in the field of Ti alloys and titanium compounds. This plot shows the temperature dependence of electrical conductivity of titanium metal and its hydrides. The electrical conductivity of titanium hydride that

exhibited metal-like temperature dependence is slightly lower than that of pure titanium and almost independent of the hydrogen content.

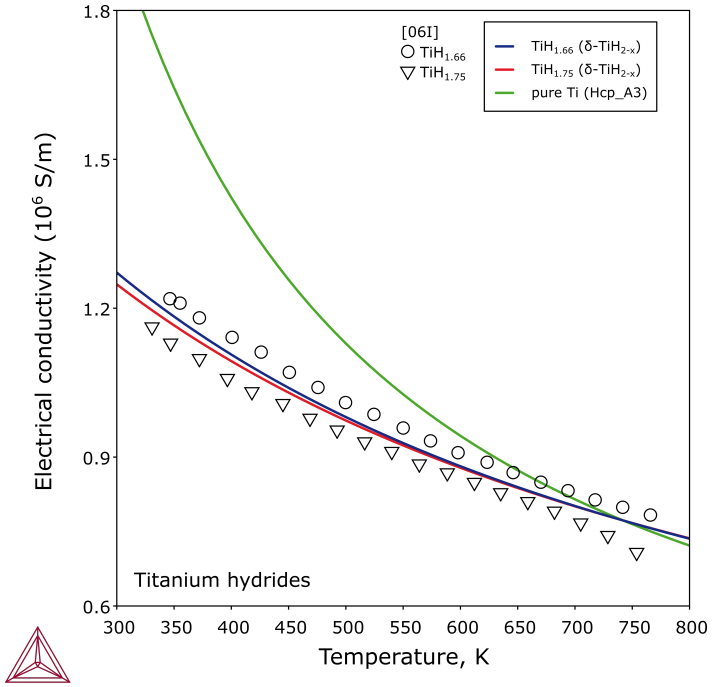

Figure 42: Calculated electrical conductivity of Ti metal and titanium hydrides.

Reference

[2006Ito] M. Ito, D. Setoyama, J. Matsunaga, H. Muta, K. Kurosaki, M. Uno, S. Yamanaka, Electrical and thermal properties of titanium hydrides. J. Alloys Compd. 420, 25–28 (2006).

Thermal Conductivity of Titanium Alloys

In the field of additive manufacturing, there are many researchers investigating titanium alloys. During the design and simulation process, it is important to have the necessary thermal conductivity data for a wide spectrum of compositions.

Using Thermo-Calc with the TCS Ti/TiAl-based Alloys Database (TCTI), you can calculate the quantities of a phase ϕ with the variable THCD (ϕ), or a system (i.e. alloy) with THCD. You can also calculate the derived quantities, i.e. thermal resistivity (THRS) and thermal diffusivity (THDF), in a similar way.

The database includes thermal conductivity starting with version 4 (TCTI4).

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

TiAl Intermetallic Compound

The γ phase is a key constituent phase for TiAl-based alloys. The plot shows calculated thermal conductivity for a TiAl intermetallic compound, which gives confidence on predictions of thermal conductivity for TiAl-based alloys when using the TCS Ti/TiAl-based Alloys Database (TCTI).

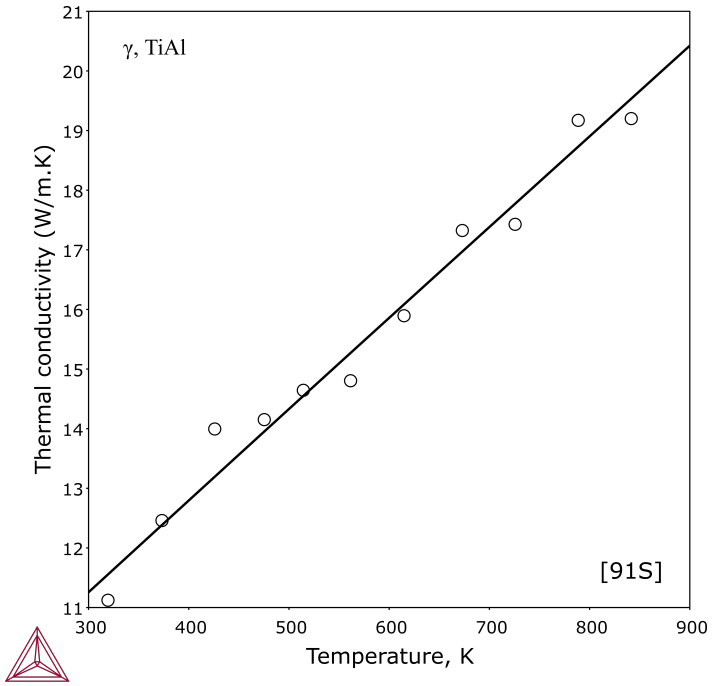

Figure 43: Calculated thermal conductivity of a TiAl intermetallic compound.

Variability in Experimental Data - An Example

During the modeling of both electrical resistivity and thermal conductivity for titanium alloys, a lot of time is spent assessing experimental data from the literature. This is critical in order to obtain reliable self-consistent descriptions of the given sub-systems, and then to be able to combine these systems and obtain predictions in multicomponent systems.

For measurements of transport properties such as electrical resistivity or thermal conductivity/diffusivity, the reported data for a single material may show significant scatter, which is generally also plagued with difficulties and measurement uncertainties.

Electrical Resistivity and Conductivity of Titanium Alloys

Common variability in the experimental data arises mainly from uncertainty of composition, unknown or ambiguous thermal history during manufacture, impurities, and so forth. This example shows some of this data scattering from the literature. A negative temperature dependence is revealed by three sets of data while the other two sets give almost constant thermal conductivity from ~500 to 2000 K.

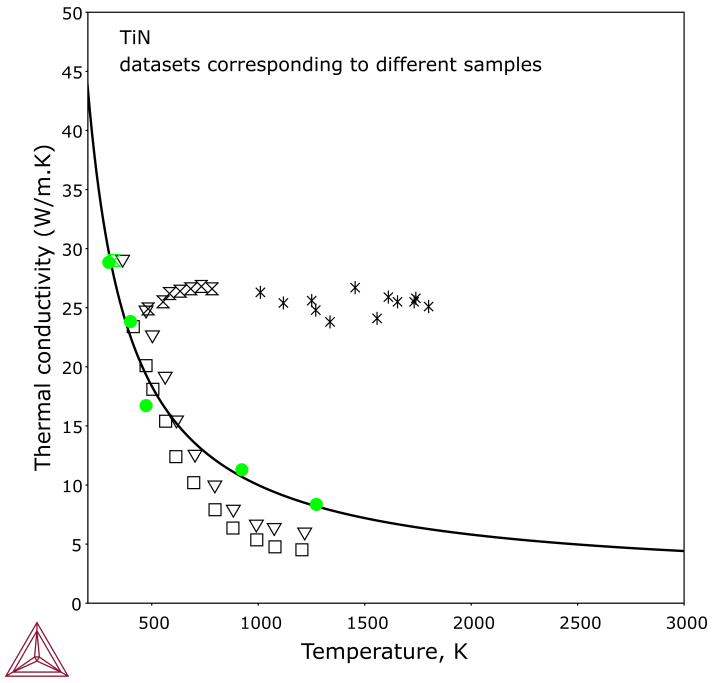

Figure 44: Calculated thermal conductivity of TiN.

Applications Using the Diffusion Module (DICTRA)

These examples use the thermodynamic TCS Ti/TiAl-based Alloys Database (TCTI) and its compatible TCS Ti-alloys Mobility Database (MOBTI) with the Add-on Diffusion Module (DICTRA).

Read more about the Diffusion Module (DICTRA) on our website. There is also a Getting Started with the Diffusion Module (DICTRA) page available. If you are in Thermo-Calc, press F1 to search the help to learn about the available settings included with the Add-on Module.

Diffusion Kinetics Simulation in BCC_A2 Ti-alloys for Biomedical Implants

BCC_A2 Ti-alloys are attractive for several biomedical applications due to their biologically safe character, good biocompatible, low Young's modulus, and high mechanical strength. The elements Nb and Zr are two important components in the BCC_A2 biomedical Ti-alloys with a low Young's modulus. However, surgeons always require the implant biomaterials with a high Young's modulus to suppress springback during surgery. The addition of element Cr can help develop novel BCC_A2 Ti-alloys with a changeable Young's modulus.

The following example shows the results from the Diffusion Module (DICTRA) simulation of a BCC_A2 Ti-0.193Zr-0.0175Cr/Ti-0.175Nb-0.0475Cr diffusion couple using the latest versions of the databases (TCTI6 and MOBTI5). The concentration profiles within the diffusion couple are simulated, with an annealing temperature 1273 K for 90000 s.

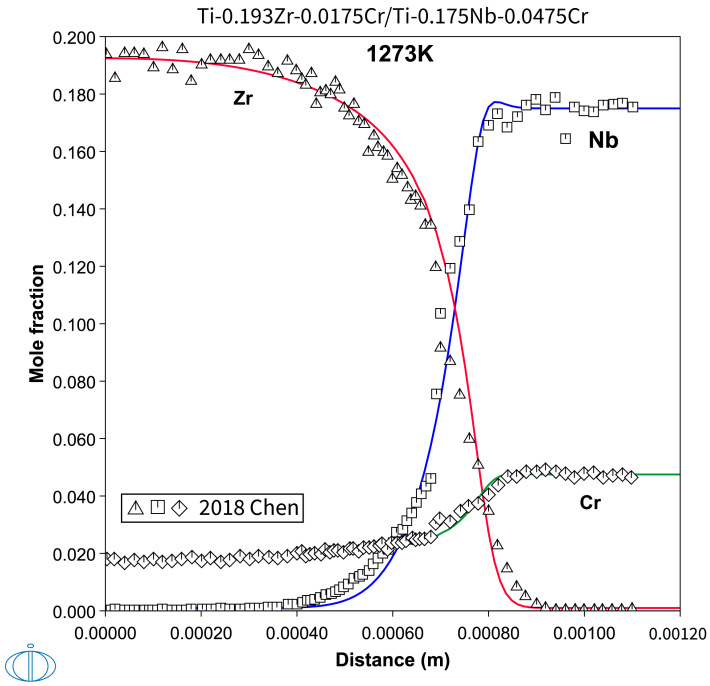

Figure 45: The simulated concentration profiles within the BCC_A2 Ti-0.193Zr-0.0175Cr/Ti-0.175Nb-0.0475Cr diffusion couple using DICTRA, with an annealing temperature 1273 K for 90000 s, and compared with the experimental data [2018Che].

Diffusivity Calculations in Ti_3Al for High Temperature Applications

The formation of Ti_3Al in Ti-alloys achieves a combination of properties that make them suitable for demanding applications in high temperature and high stress environments. These properties include improved high temperature strength, oxidation resistance, increased creep resistance, enhanced structural stability, and balanced mechanical properties. The development of such intermetallic compounds as structural materials inevitably requires knowledge of relevant diffusion data. Attention to such investigations is attractive not only for accumulating experimental data but also for gaining a deeper insight into the underlying microscopic diffusion mechanisms.

The following example shows the results from the simulation of tracer diffusivities of the substitutional elements Ni, Ti, Al, and Nb, as well as the interstitial element, H, in the compound Ti_3Al as a function of temperature.

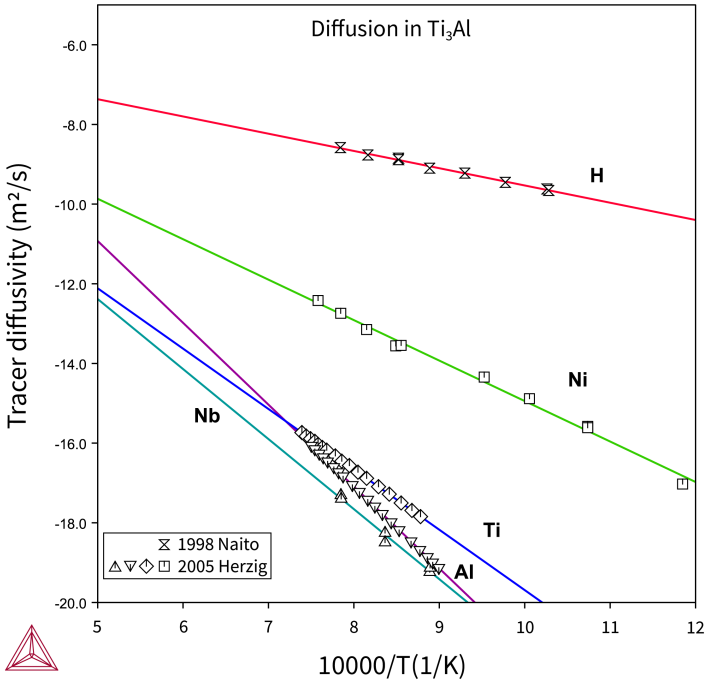

Figure 46: The simulated tracer diffusivities of substitutional elements Ni, Ti, Al, and Nb, as well as the interstitial element H, in the compound Ti_3Al as a function of temperature, and compared with the experimental data [1998Nai; 2005Her] .

References

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