TCS Mo-based Alloys Database (TCMO)

Examples Collection

Document created 6/12/2024

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 Mo-based Alloys Database (TCMO) 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 Mo-based Alloys Database (TCMO) 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 Mo-based Alloys Database (TCMO) 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 Molybdenum-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.

TCMO Validation Examples

In this section:

Phase Composition of Some Mo-Si-B Series Alloys

The multiphase composite Mo-based alloys are candidate materials to replace Ni-based superalloys that generally operate at temperatures below 1200 °C. To achieve the optimal combinations of strength, fracture toughness, and oxidation resistance, knowledge of phase relations between the ductile BCC solid solution and intermetallic compounds such as Mo_5SiB_2 (T2), Mo_3Si, Mo_5Si_3 (T1) and $D8_8$ (Ti_5Si_3) is crucial.

The TCS Mo-based Alloys Database (TCMO) can be used to predict the phase stability and compositions for a given chemistry, which is the prerequisite for Mo-based alloy design.

Mo-Ti-Si-B Calculated Phase Compositions

The quaternary Mo-Ti-Si-B alloys are expected to exhibit superior performance compared to the ternary Mo-Si-B alloys due to the introduction of the Ti_5Si_3 phase. The table confirms that when using the TCS Mo-based Alloys Database (TCMO) database, the predicted stable phases and phase compositions for 10 Mo-Ti-Si-B alloys at 1600 °C are in good agreement with the experimental results from [2005Yan].

Alloy chemistry, at.%			*Ti composition in each phase, at.%*									
			T2		*Mo_3Si*		*BCC*		*T1*		*Ti_5Si_3*	
B	*Si*	*Ti*	*Exp.*	*Calc.*	*Exp.*	*Calc.*	*Exp.*	*Calc.*	*Exp.*	*Calc.*	*Exp.*	*Calc.*
19	11	10	12.9±1	11.8	9.3±1	14.3	1±0.5	1.4				
		20	22.7±1.5	22.0	22.1±2	23.3	14.4±3	11.0				
		30	29.1±2	28.7			33.6±3	32.3			52.1±1	50.4
9	18	28.5	26±2	26.4	33.5±2	27.2	24±1	24.1	41±1.5	39.4		
		32.5	26.5±2	27.4			27±1	27.7	42.3±2	40.4	49.2±1	48.9
		35	26.7±2	27.5			27.8±1	28.1			50.5±1	49.0
		37.5	27.2±2	28.9			35±1	33.0			53±1	51.0
10	10	25	27±3	26.2	30±2	27.0	23.8±1	23.2				
		27.5	27.8±3.5	26.8			26.4±0.4	25.5	43±3	40.0		
		30	29±3	27.6			29.5±1	28.2			50±1	49.1

Reference

[2005Yan] Y. Yang, Y. A. Chang, L. Tan, W. Cao, Multiphase equilibria in the metal-rich region of the Mo–Ti–Si–B system: thermodynamic prediction and experimental validation. Acta Mater. 53, 1711–1720 (2005).

Effect of Alloying Elements on Phase Stability

The TCS Mo-based Alloys Database (TCMO) can be used to examine the effect of alloying elements on phase stability.

Ti, Zr, and Hf are potential BCC stabilizers for the Mo-Si-B based alloys. It is important to have a better understanding of how these alter the phase equilibria among the three base phases (BCC, T2, and Mo_3Si) and how it introduces new phases.

Figure 1 indicates that at 1600 °C the addition of Ti to the base composition Mo-12.5Si-8.5B (at.%) stabilizes BCC and T1 at the expense of Mo_3Si. When Ti content exceeds 30 at.%, the Ti_5Si_3 phase starts to form at the expense of the T1 phase. The calculated phase compositions for the Mo-12.5Si-8.5B-27.5Ti (at.%) alloy are consistent with the experimental measurements from [2010Yan].

By contrast, Figure 2 shows that the introduction of Zr to the Mo-12.5Si-8.5B (at.%) alloy leads to the formation of the MoSiZr phase. The calculated phase compositions for the Mo-12.5Si-8.5B-3Zr (at.%) alloy agree well with the experimental measurements from [2010Yan].

Similarly, Hf also results in the appearance of the MoSiHf phase as shown in Figure 3. The calculated phase compositions for the Mo-12.5Si-8.5B-6Hf (at.%) alloy are in good accordance with the experimental measurements from [2010Yan].

Mo-Si-B-Ti

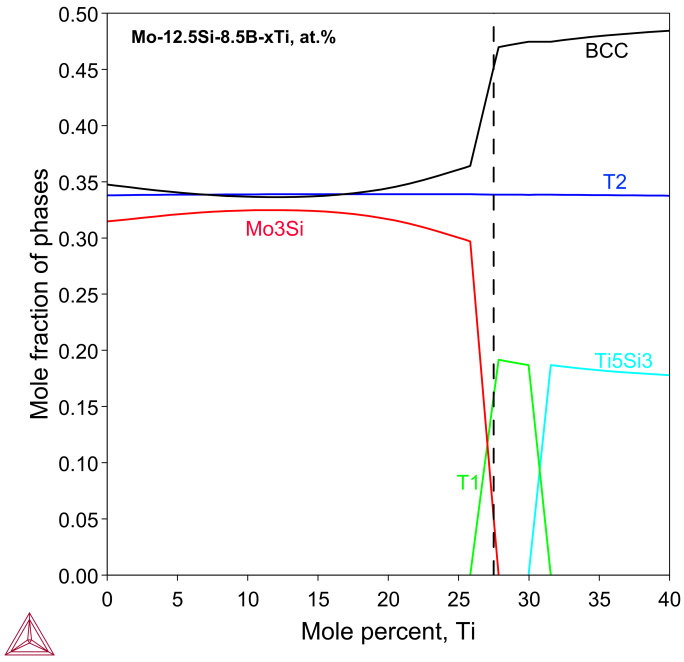

Figure 1: Calculated phase fractions as a function of Ti concentration in the Mo-12.5Si-8.5B-xTi (at.%) alloys at 1600 °C. The dashed line marks the experimentally investigated composition where x = 27.5.

Calculated phase compositions for the Mo-12.5Si-8.5B-27.5Ti (at.%) alloy at 1600 °C compared with experimental data from [2010Yan].

Phase	BCC, at.%		Mo_3Si, at.%		T2, at.%		T1, at.%	
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.
Mo	69.5	73.5	47.7	47.8	35.0	36.1	24.6	23.1
Ti	24.5	24.1	29.9	27.2	29.0	26.4	38.7	39.4
Si	2.3	2.3	22.4	25.0	13.5	12.5	36.7	37.5
B	3.7*	0.1	~0*	0	22.5*	25.0	~0*	0
* B content was not accurately measured in the experiment								

Mo-Si-B-Zr

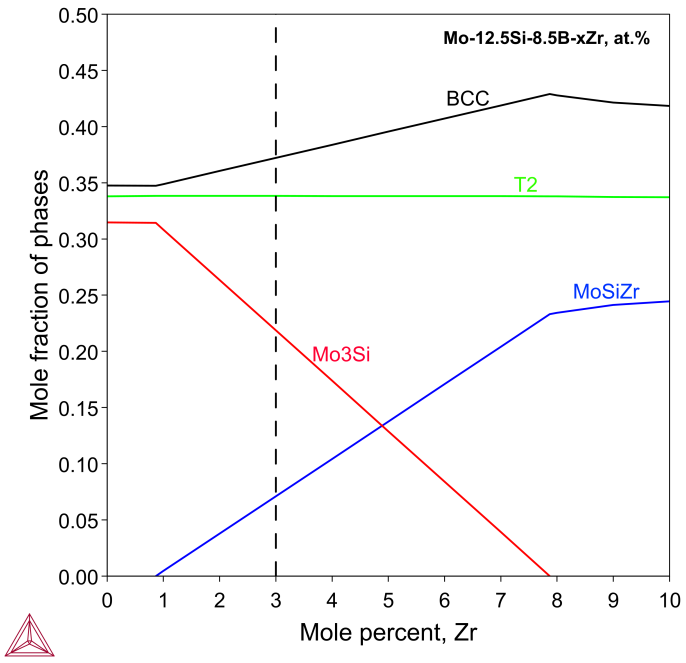

Figure 2: Calculated phase fractions as a function of Zr concentration in the Mo-12.5Si-8.5B-xZr (at.%) alloys at 1600 °C. The dashed line marks the experimentally investigated composition where x = 3.

Calculated phase compositions for the Mo-12.5Si-8.5B-3Zr (at.%) alloy at 1600 °C compared with experimental data from [2010Yan].

Phase	BCC, at.%		Mo_3Si, at.%		T2, at.%		T1, at.%	
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.
Mo	90.0	98.6	74.0	74.5	58.0	60.5	36.4	36.0
Zr	0.3	0.1	0.5	0.5	2.0	2.0	31.3	30.7
Si	3.0	1.2	24.5	25.0	12.0	12.5	32.4	33.3
B	6.7*	0.1	~0*	0	28.0*	25.0	~0*	0
* B content was not accurately measured in the experiment								

Mo-Si-B-Hf

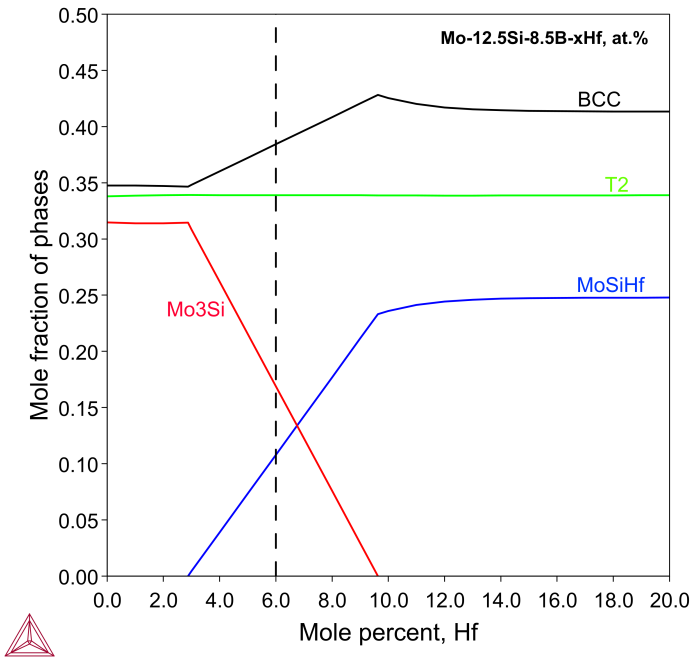

Figure 3: Calculated phase fractions as a function of Hf concentration in the Mo-12.5Si-8.5B-xHf (at.%) alloys at 1600 °C. The dashed line marks the experimentally investigated composition where x = 6.

Calculated phase compositions for the Mo-12.5Si-8.5B-6Hf (at.%) alloy at 1600 °C compared with experimental data from [2010Yan].

Phase	BCC, at.%		Mo_3Si, at.%		T2, at.%		T1, at.%	
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.
Mo	88.0	98.6	74.0	73.6	57.0	55.4	35.0	35.9
Hf	1.4	0.1	1.3	1.4	7.0	7.1	30.5	30.8
Si	3.1	1.2	24.7	25.0	14.0	12.5	34.5	33.3
B	7.5*	0.1	~0*	0	22.0*	25.0	~0*	0
* B content was not accurately measured in the experiment								

Reference

[2010Yan] Y. Yang, H. Bei, S. Chen, E. P. George, J. Tiley, Y. A. Chang, Effects of Ti, Zr, and Hf on the phase stability of Mo_ss + Mo3Si + Mo5SiB2 alloys at 1600°C. Acta Mater. 58, 541–548 (2010).

Phase Fraction of TiC-added Mo-Si-B Alloys

The TCS Mo-based Alloys Database (TCMO) database can be used to study the phase fraction of TiC-added Mo-Si-B alloys.

Due to its high melting point and low density, TiC can act as an excellent strengthening phase in Mo-Si-B alloys. Moreover, the primary TiC phase contributes to a continuous BCC matrix and thus improves the fracture toughness.

Figure 4 shows that in the Mo-Si-B-TiC series alloys where *x*(Mo)=0.65 and *x*(Si):*x*(B)=0.5, the increase of the TiC content increases the volume fractions of BCC and TiC, while decreasing those of T2 and Mo_2C. Such a trend was confirmed by experiments from [2014Miy].

A similar trend is predicted for the Mo-Si-B-TiC series alloys where *x*(Mo)=0.7 and *x*(Si):*x*(B)=0.5 (as shown in Figure 5). Deviations between the calculated and experimental volume fractions of phases exist for the TiC content of 7.5 and 12.5 at.%, which may come from the weak contrast difference between different phases or the insufficient annealing time to reach complete equilibrium.

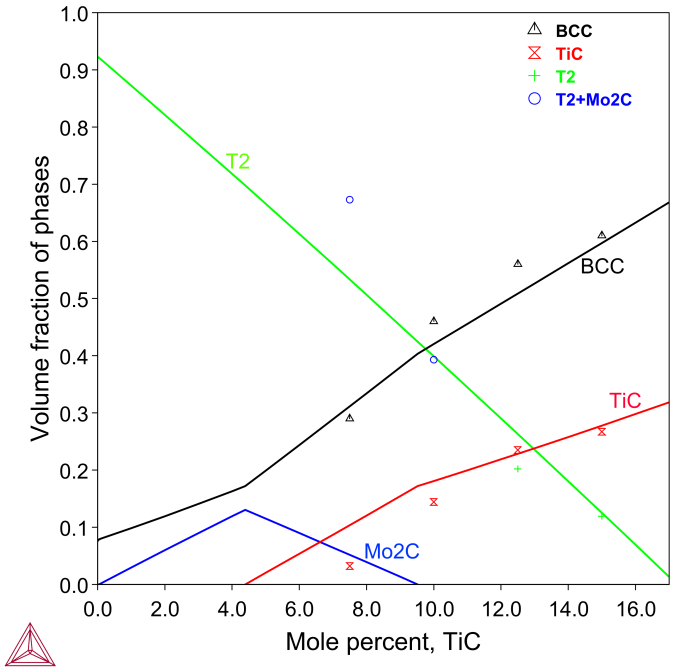

Figure 4: Calculated volume fraction of phases for the Mo-Si-B-TiC series alloys where x(Mo)=0.65, x(Si):x(B)=0.5 at 1800 °C. Experimental data are from [2014Miy].

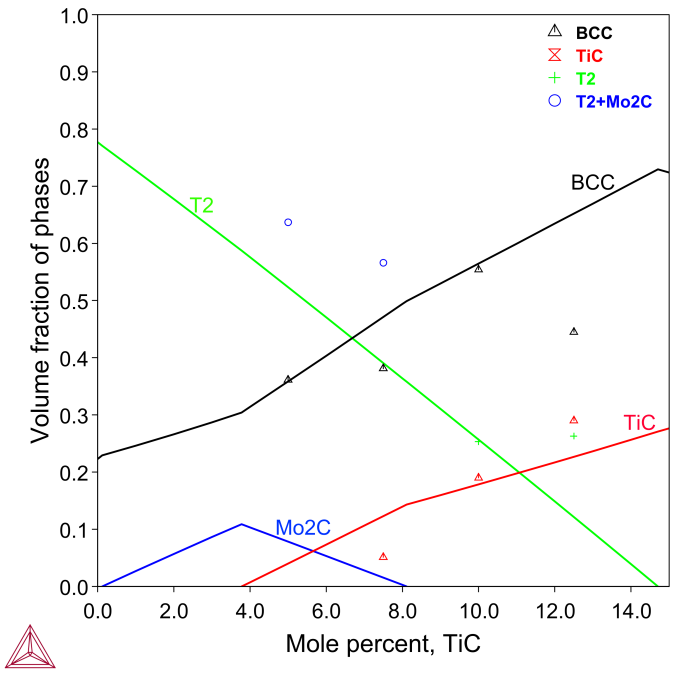

Figure 5: Calculated volume fraction of phases for the Mo-Si-B-TiC series alloys where x(Mo)=0.7, x(Si):x(B)=0.5 at 1800 °C. Experimental data are from [2013Miy].

Reference

[2014Miy] S. Miyamoto, K. Yoshimi, S.-H. Ha, T. Kaneko, J. Nakamura, T. Sato, K. Maruyama, R. Tu, T. Goto, Phase Equilibria, Microstructure, and High-Temperature Strength of TiC-Added Mo-Si-B Alloys. Metall. Mater. Trans. A. 45, 1112–1123 (2014).

Solidification Path of TiC-added Mo-Si-B Alloys

For TiC-added Mo-Si-B alloys, the primary phase is considerably influenced by the alloy composition. The TCS Mo-based Alloys Database (TCMO) can also predict the solidification path for these alloys. For example, in the Mo-1.7Si-3.3B-15TiC (at.%) alloy, TiC solidifies first, followed by the BCC+TiC eutectic. By contrast, in the Mo-6.7Si-13.3B-7.5TiC (at.%) alloy, the primary solidification phase becomes T2. The predicted solidification paths and primary solidification phases are consistent with the experimental observation from [2014Miy].

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.

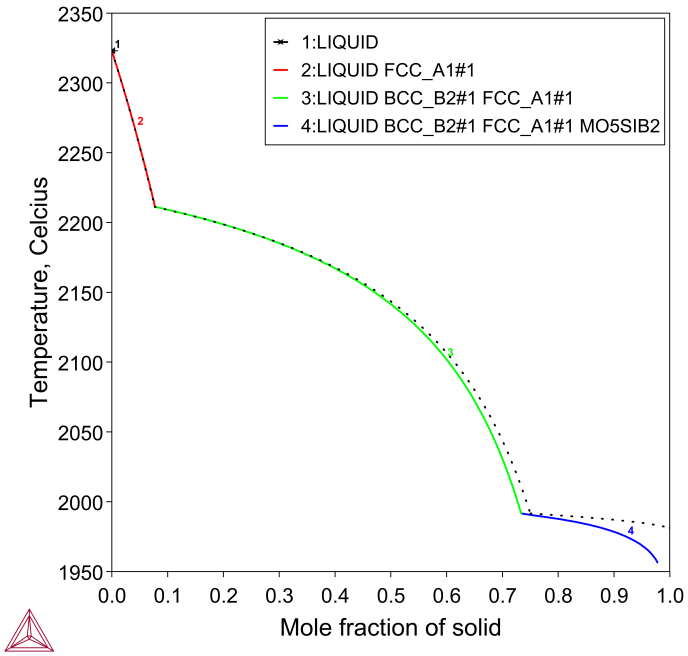

Figure 6: Equilibrium solidification and Scheil solidification simulations of the Mo-1.7Si-3.3B-15TiC (at.%) alloy. The predicted solidification path and primary solidification phase are consistent with the experimental observation from [2014Miy].

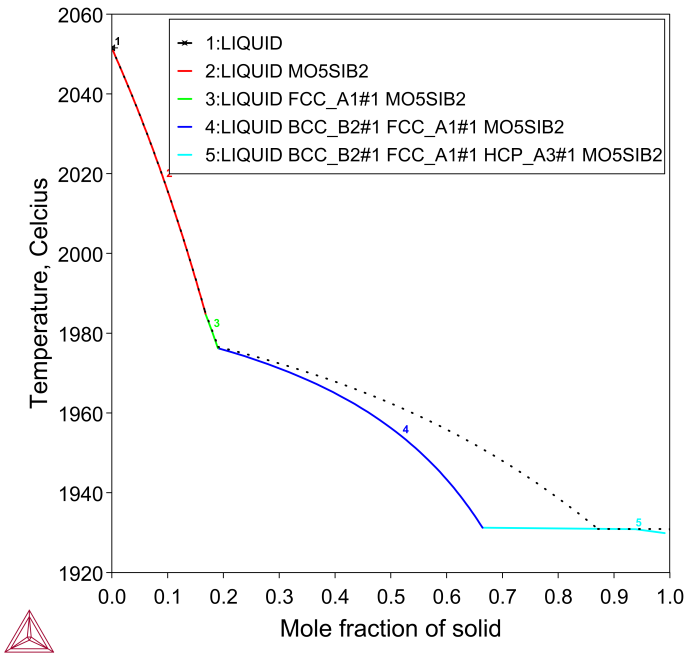

Figure 7: Equilibrium solidification and Scheil solidification simulations of the Mo-6.7Si-13.3B-7.5TiC (at.%) alloy. The predicted solidification path and primary solidification phase are consistent with the experimental observation from [2014Miy].

Reference

[2014Miy] S. Miyamoto, K. Yoshimi, S.-H. Ha, T. Kaneko, J. Nakamura, T. Sato, K. Maruyama, R. Tu, T. Goto, Phase Equilibria, Microstructure, and High-Temperature Strength of TiC-Added Mo-Si-B Alloys. Metall. Mater. Trans. A. 45, 1112–1123 (2014).

Growth of an Mo_5Si_3 Layer in Mo/$MoSi_2$ Coatings at High Temperatures

This example uses the thermodynamic TCS Mo-based Alloys Database (TCMO) and its compatible TCS Mo-based Alloys Mobility Database (MOBMO) with the Add-on Diffusion Module (DICTRA) to study layer growth in coatings at high temperatures.

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.

To enhance the high-temperature oxidation resistance of Mo-based alloys, applying a $MoSi_2$ ceramic coating on the substrates is highly effective because it forms protective SiO_2 scales on the coating's surface. Moreover, since Si atoms diffuse into Mo substrates more rapidly than Mo atoms, this inward diffusion of Si results in the formation and growth of a Mo_5Si_3 layer.

The following example shows the results from the Diffusion Module (DICTRA) simulation of Mo substrate joined with an $MoSi_2$ coating material by using the most recent versions of the Mo-based databases (TCMO1 and MOBMO1). The growth of the Mo_5Si_3 layer between the Mo substrate and $MoSi_2$ coating is simulated using the homogenization model, with annealing temperatures ranging from 1473 K to 1773 K for 30 s.

The thickness of Mo_5Si_3 was estimated based on the Mo concentration profiles in the Mo/$MoSi_2$/Mo_5Si_3 diffusion couple at different times and temperatures. In this case, TC-Python was used to generate the plot shown in Figure 8.

Read more about TC-Python and its capabilities on our website. Scroll to the bottom of the page to access several resources such as videos, publications, blogs, documentation, and much more.

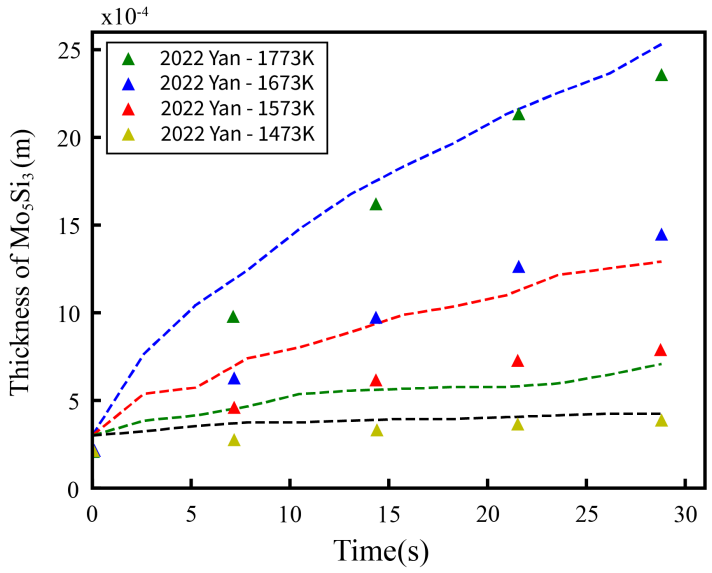

Figure 8: The simulated growth of Mo_5Si_3 layer between Mo substrate and $MoSi_2$ layer using the homogenization model implemented in the Diffusion Module (DICTRA), with annealing temperatures ranging from 1473 K to 1773 K with experimental data from [2022Yan].

Reference

[2022Yan] J. Yan, Y. Z. Lin, Y. Wang, J. Qiu, F. Wan, C. Song, Refractory WMoNbVTa high-entropy alloy as a diffusion barrier between a molybdenum substrate and MoSi2 ceramic coating. Ceram. Int. 48, 11410–11418 (2022).

Growth of an Mo_2C Layer on Mo Surface During Carburization

This example uses the thermodynamic TCS Mo-based Alloys Database (TCMO) and its compatible TCS Mo-based Alloys Mobility Database (MOBMO) with the Add-on Diffusion Module (DICTRA) to study layer growth on a surface during carburization.

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.

The inward diffusion of carbon into Mo-based alloys during carburization can lead to the formation of Mo carbides due to the low solubility of carbon in the metal matrix. Within the Mo_2C layer, carbon diffusivity is significantly higher than that of molybdenum, resulting in the primary inward growth of the Mo_2C layer. Consequently, this growth process can be considered as occurring in a closed system.

The following example shows the results from the Diffusion Module (DICTRA) simulation of pure Mo metal exposed to a carbon dioxide-containing gas atmosphere by using the most recent versions of the Mo-based databases (TCMO1 and MOBMO1).

The growth of Mo_2C layer is simulated with a boundary condition of `acrC=1` using the moving boundary model, with a temperature range of 1273-1673 K for 64 h.

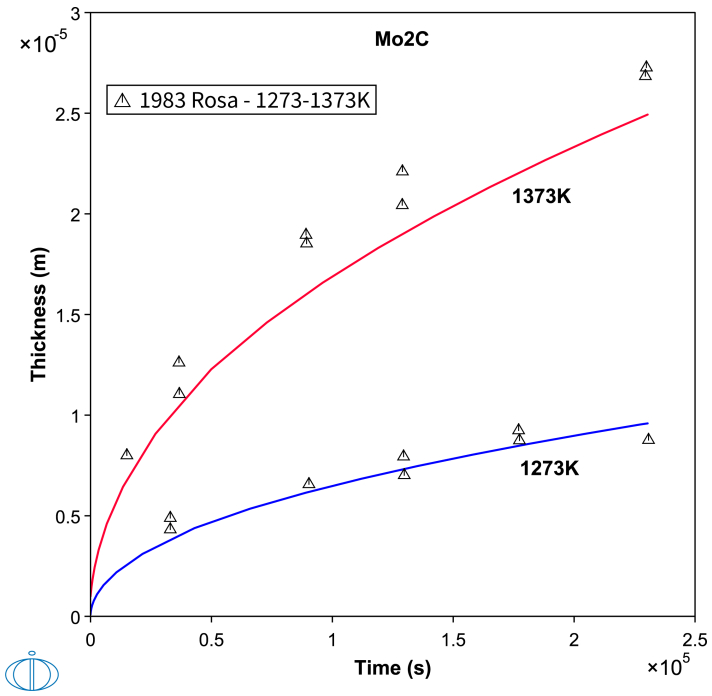

Figure 9: The simulated growth of Mo_2C layer on the Mo surface with a boundary condition of acr(C)=1 using the moving boundary model, with a temperature range of 1273-1373 K for 64 h, compared with the experimental data from [1983Ros].

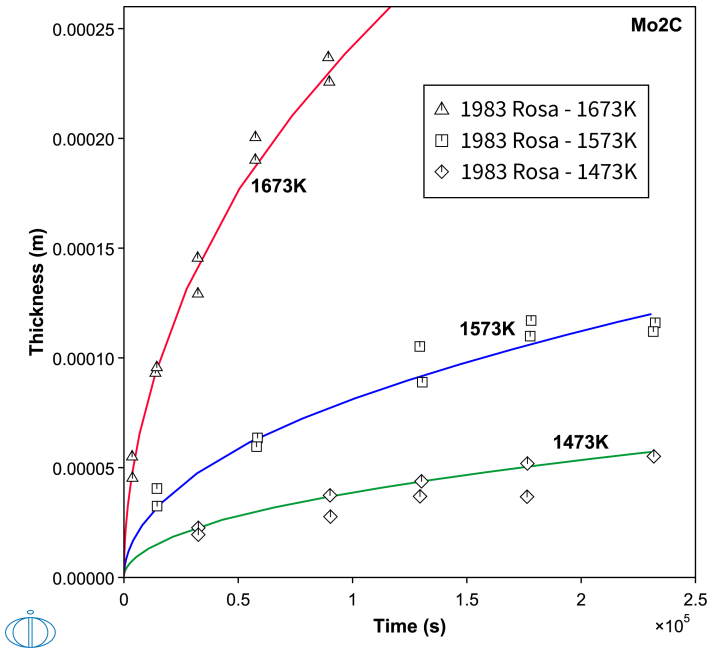

Figure 10: The simulated growth of Mo_2C layer on the Mo surface with a boundary condition of acr(C)=1 using the moving boundary model, with a temperature range of 1473-1673 K for 64 h, compared with the experimental data from [1983Ros].

Reference

[1983Ros] C. J. Rosa, Carbon diffusion in Mo_2C as determined from carburization of Mo. Metall. Trans. A. 14, 199–202 (1983).

TCMO Calculation Examples

In this section:

Binary Phase Diagrams

You can use the TCS Mo-based Alloys Database (TCMO) to plot binary phase diagrams in Thermo-Calc. Each binary system is critically assessed to reproduce the phase diagram and thermodynamic properties data available in the literature.

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

The examples shown here are important sub-systems of the Mo-Si-B based alloys. Mo_3Si, Mo_5Si_3, and Ti_5Si_3 are also major phases that influence the performance of the Mo-Si-B based alloys.

Mo-Si

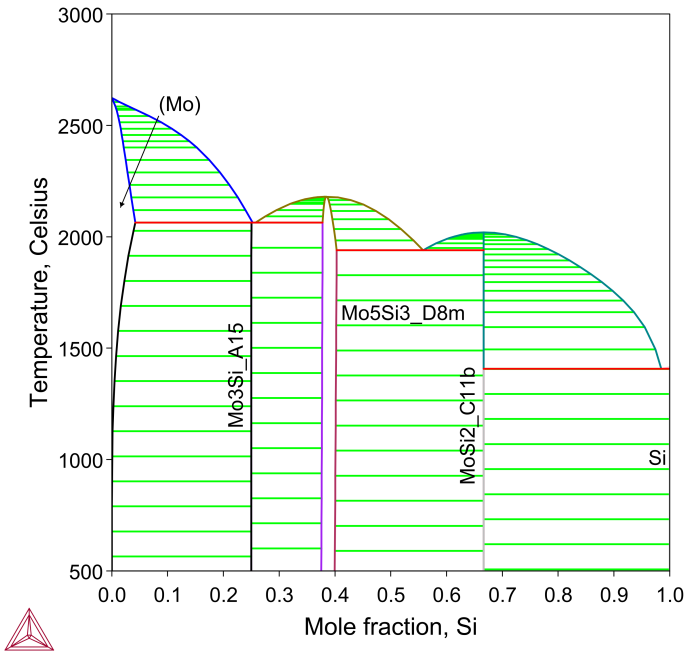

Figure 11: Calculated Mo-Si phase diagram [2000Liu].

Ti-Si

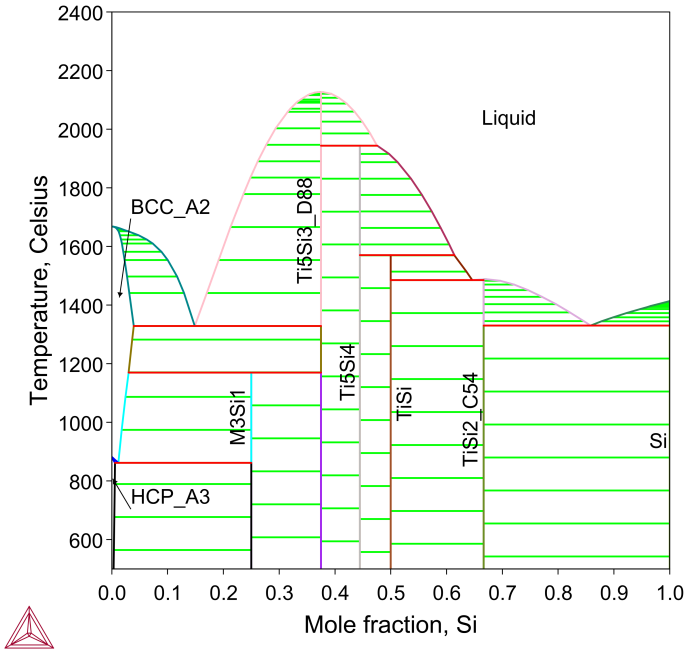

Figure 12: Calculated Ti-Si phase diagram [2000Du]. The Ti5Si3_D88 phase is simplified as stoichiometric in the database.

References

[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).

[2000Liu] Y. Liu, G. Shao, P. Tsakiropoulos, Thermodynamic reassessment of the Mo–Si and Al–Mo–Si systems. Intermetallics. 8, 953–962 (2000).

Ternary Phase Diagrams

You can use the TCS Mo-based Alloys Database (TCMO) to plot ternary phase diagrams in Thermo-Calc. Each ternary system is critically assessed to reproduce the phase diagram and thermodynamic properties data available in the literature. The following examples show a selection of the key 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.

B-Mo-Si: Isothermal Section and Liquidus Projection

B-Mo-Si is the base system for Mo-based alloys frequently investigated in the literature, where the T2 (Mo_5SiB_2) phase forms and the T1 (Mo_5Si_3) phase dissolves a certain amount of boron. The B-Mo-Si ternary system has been assessed to also consider the experimentally observed primary solidification phases.

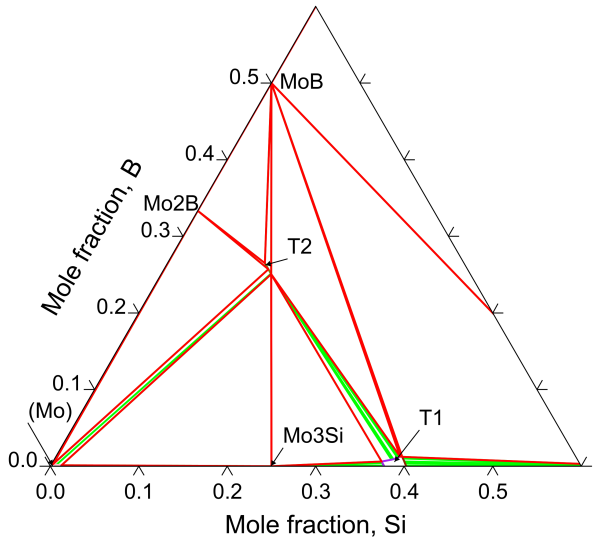

Figure 13: Calculated B-Mo-Si isothermal section on the Mo-rich corner at 1600 °C.

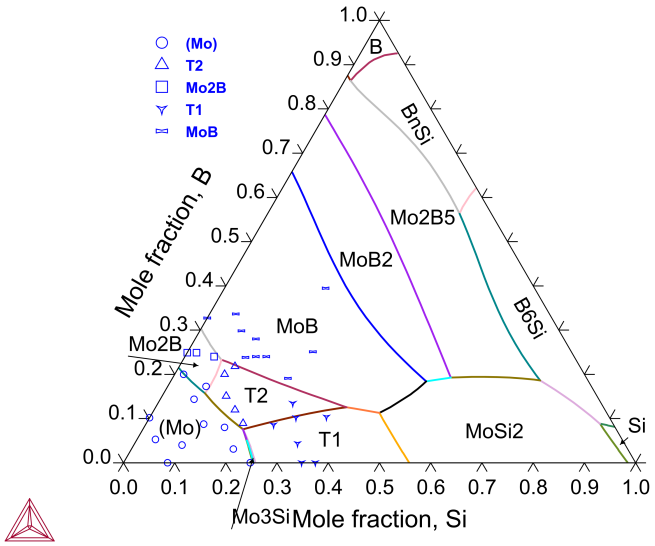

Figure 14: Calculated B-Mo-Si liquidus projection compared with experimental data from [2005Yan].

Mo-Si-Ti: Isothermal Sections and Liquidus Projection

Titanium (Ti) is an important alloying element in the Mo-Si-B based alloys since Ti exhibits a large solubility in the Mo_3Si and Mo_5Si_3 phases and the Ti_5Si_3 phase plays a critical role in tuning the alloys' properties. The Mo-Si-Ti ternary system has been assessed to reproduce the experimental isothermal sections and liquidus projection.

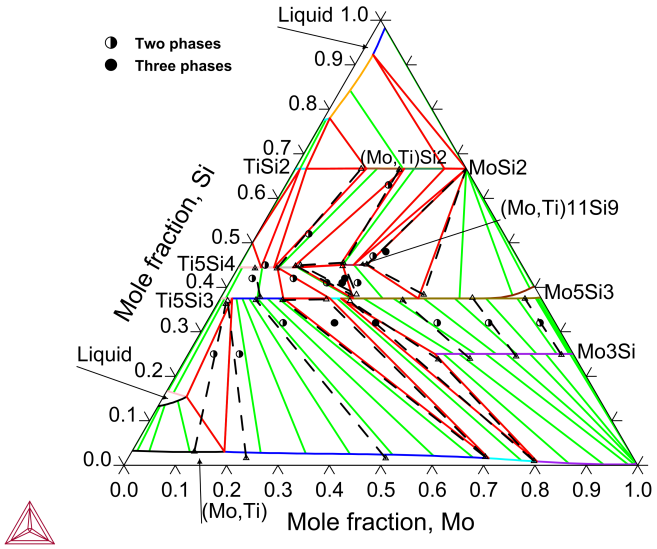

Figure 15: Calculated Mo-Si-Ti isothermal section at 1425 °C compared with experimental data from [2003Yan]. The dashed lines represent experimentally measured tie-lines or tie-triangles.

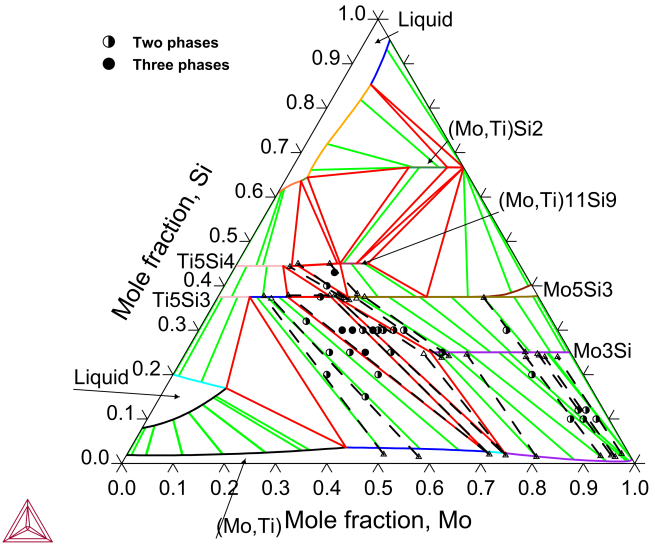

Figure 16: Calculated Mo-Si-Ti isothermal section at 1600 °C compared with experimental data from [2003Yan]. The dashed lines represent experimentally measured tie-lines or tie-triangles.

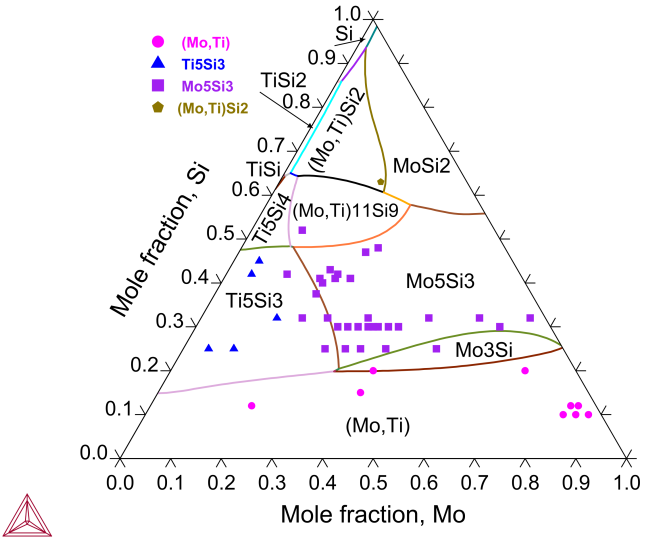

Figure 17: Calculated Mo-Si-Ti liquidus projection compared with experimental data from [2003Yan].

Cr-Mo-Si: Isothermal Sections and Liquidus Projection

Chromium (Cr) is another important alloying element in the Mo-Si-B based alloys where the low-temperature Cr_5Si_3 phase shares the same structure as Mo_5Si_3 and a continuous series of solid solution exists between Mo_3Si and Cr_3Si. The Cr-Mo-Si ternary system has been assessed to reproduce the experimental isothermal sections and liquidus projection.

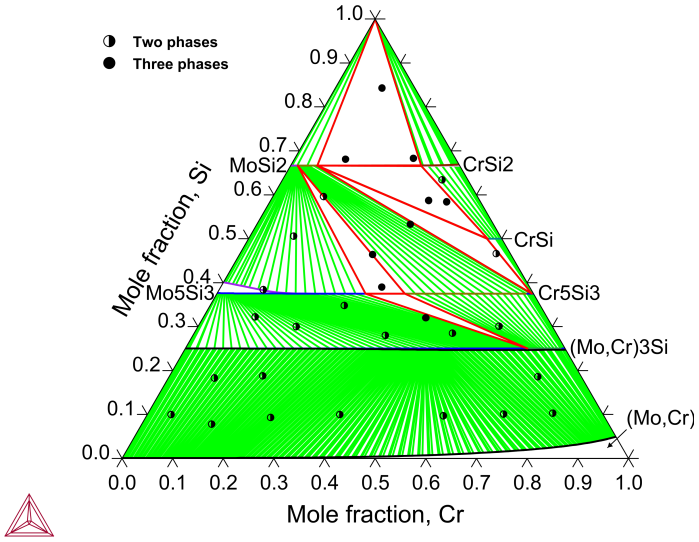

Figure 18: Calculated Cr-Mo-Si isothermal section at 1000 °C compared with experimental data from [2022Wu].

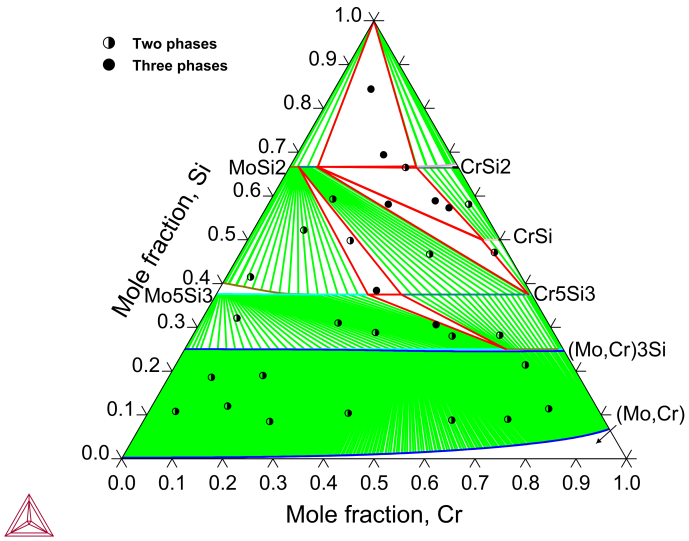

Figure 19: Calculated Cr-Mo-Si isothermal section at 1200 °C compared with experimental data from [2022Wu].

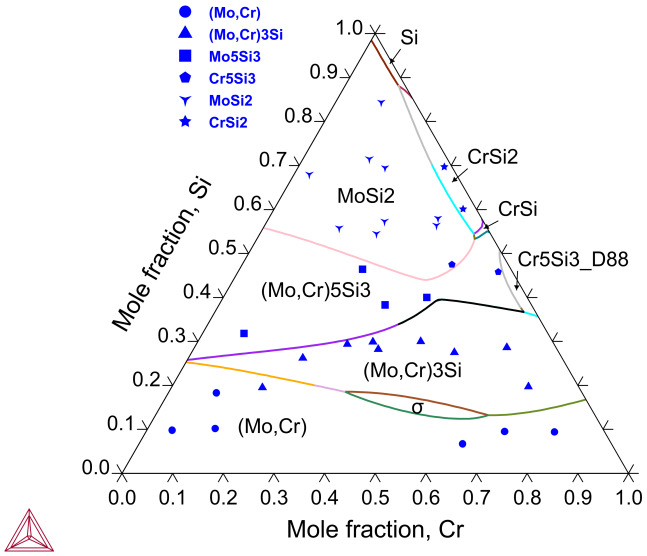

Figure 20: Calculated Cr-Mo-Si liquidus projection compared with experimental data from [2022Wu].

C-Mo-Si: Isothermal Section

Carbon (C) can be added to the Mo-Si-B based alloys to introduce desired carbide phases. Moreover, the introduction of C always leads to the formation of the $D8_8$ phase in the M-Si-C (M: Metal element) ternary systems, for example, in C-Mo-Si.

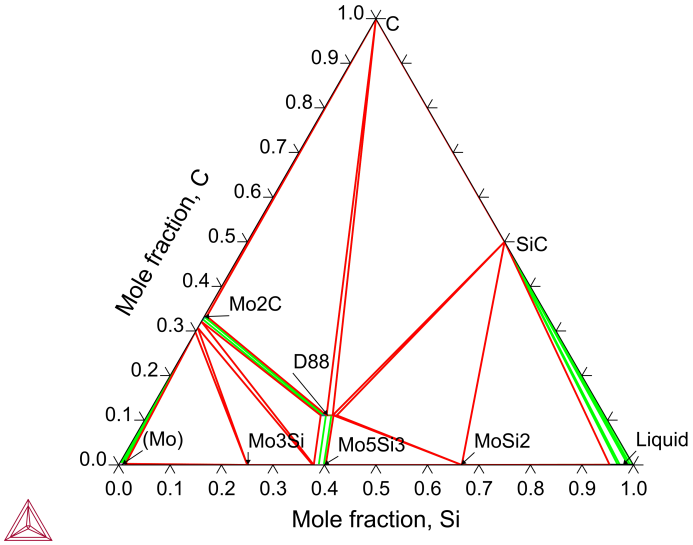

Figure 21: Calculated C-Mo-Si isothermal section at 1600 °C.

References

[2003Yan] Y. Yang, Y. A. Chang, L. Tan, Y. Du, Experimental investigation and thermodynamic descriptions of the Mo–Si–Ti system. Mater. Sci. Eng. A. 361, 281–293 (2003).

[2005Yan] Y. Yang, Y. A. Chang, Thermodynamic modeling of the Mo–Si–B system. Intermetallics. 13, 121–128 (2005).

[2022Wu] H. Wu, C. Li, C. Guo, Z. Du, Experimental determination of the isothermal sections and the liquidus surface projection of the Mo-Si-Cr ternary system. J. Alloys Compd. 922, 166164 (2022).

Applications Using the Diffusion Module (DICTRA)

This example uses the thermodynamic TCS Mo-based Alloys Database (TCMO)and its compatible TCS Mo-based Alloys Mobility Database (MOBMO) 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.

Intermetallic Formation on Diffusion Behavior for Zr-Mo Alloys

This example examines the impact of Mo_2Zr intermetallic formation on diffusion behavior in Zr-Mo alloys used for nuclear applications

Zr-Mo alloys are widely used as nuclear fuel cladding materials and reactive structural materials due to their high density, radiation resistance, high strength, and favorable oxidation behavior with oxygen. The formation of intermetallic compound Mo_2Zr enhances the alloy's strength and radiation resistance. However, the diffusion processes within Mo_2Zr and its solid solutions can interact, impacting the overall material properties. Therefore, studying and analyzing the diffusion behavior in the Zr-Mo binary system is crucial to understanding and optimizing the performance of the alloy.

The following example shows the results from the Diffusion Module (DICTRA) simulation of growth of Mo_2Zr compound layer in the Mo/Zr diffusion couple in the temperature range of 1573 K to 1773 K, using the latest versions of the databases (TCMO1 and MOBMO1).

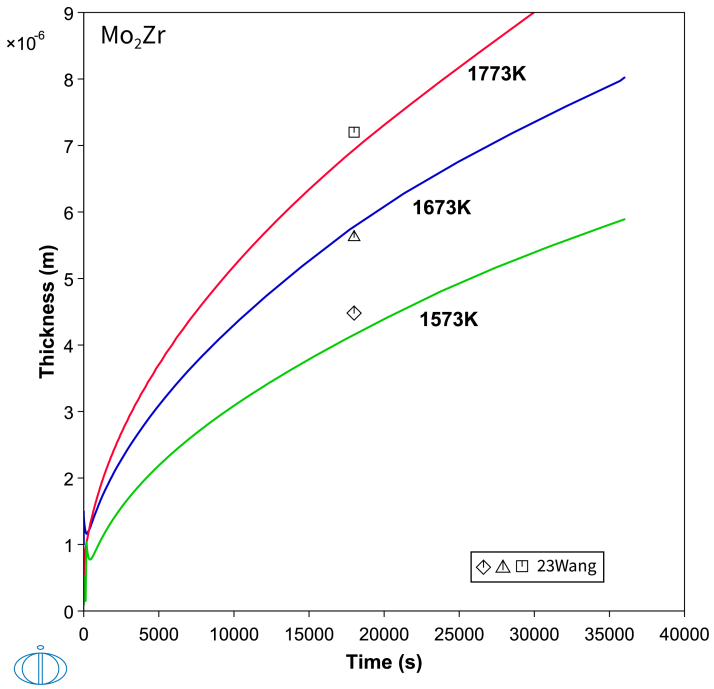

Figure 22: The simulated growth of Mo_2Zr layer in the Mo/Zr diffusion couple in the temperature range of 1573 K to 1773 K for 10 h, compared with the experimental data.

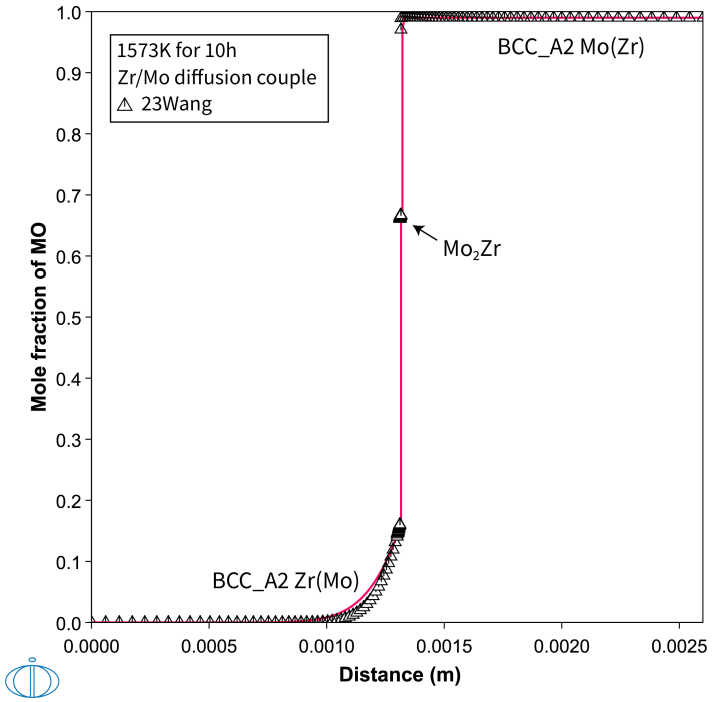

Figure 23: The simulated concentration profiles of Mo in the Zr/Mo_2Zr/Mo diffusion couple at 1573 K for 10 h, using both the thermodynamic and kinetic Mo-based databases compared with the experimental data [2023Wan].

Reference

[2023Wan] 1. K. Wang, X. Liu, T. Liu, C. He, J. Liu, Interdiffusion in Zr-Mo/W Intermetallics. Appl. Sci. 13, 6375 (2023).