Thermo-Calc Software

TCS High Entropy Alloys Database (TCHEA)

Validation and Calculation Examples Collection

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Contents

About the Database Examples

The *Validation and Calculation Examples Collection* that is available for many databases demonstrates both the *validity* of the database itself as well as demonstrates 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.

About the TCHEA Examples

For the studies related to high entropy alloys (HEAs), this selection of examples demonstrate the calculation capacity of available tools such as the thermodynamic and properties databases, the kinetic databases, and the many features available in Thermo-Calc both in Graphical and Console Mode.

The TCHEA Calculation Examples and TCHEA Validation Examples are performed using the thermodynamic database TCS High Entropy Alloys Database (TCHEA) and the Thermo-Calc software. These examples focus on the equilibrium calculations, especially the stability of primary phases.

This collection includes the calculations of various thermodynamic and physicochemical properties and different types of process simulations. Classical calculations on equilibrium phase stabilities of FCC, BCC, and HCP MEAs and HEAs are first demonstrated. It followed by the examples on other properties accessible through calculations using Thermo-Calc (and Add-on Modules). These properties of HEAs include density, thermal conductivity, electrical resistivity, viscosity, surface tension and yield strength. In the end, different simulations are demonstrated include solidification process, diffusion and precipitation.

The TCHEA database is a key materials genome for the design of novel HEAs with superior mechanical and physicochemical properties by integrated computational materials engineering (ICME) method. Solidification process during the casting and phase transformations such as precipitations during annealing can be simulated using TCS High Entropy Alloys Database (TCHEA)and the TCS High Entropy Alloy Mobility Database (MOBHEA) using the advanced features available with Add-on Modules in Thermo-Calc, for example using the Diffusion Calculator or Precipitation Calculator with the Diffusion Module (DICTRA) or Precipitation Module (TC-PRISMA), respectively.

TCS High Entropy Alloys Database (TCHEA) 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 High Entropy Alloys Database (TCHEA) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, phases and models. It also includes details about the thermophysical and elastic properties data (e.g. viscosity, surface tension, etc.), a list of the included elements, and summaries of the database revision history by version.
- The *TCS High Entropy Alloys Database (TCHEA) Validation and Calculation 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 High Entropy Alloys Databases page on our website where you can access a Validation and Calculation Examples Collection and the Technical Information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to high entropy alloys and the Refractory Alloys Solutions page on our website, that includes links to resources such as examples, publications, and more.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of all the binary systems and many ternary systems. A hybrid approach of experiments, first-principal calculations and CALPHAD modeling has been used to obtain reliable thermodynamic descriptions of the BCC, FCC and HCP solutions. That enables predictions to be made for multicomponent alloy systems, especially for HEAs.

The extrapolation to higher-order systems helps to understand the phase equilibria in HEAs, so as to predict the phase formation, phase fractions and phase compositions or to calculate the driving force of forming a phase. All necessary molar volume data and thermal expansion data are assessed or estimated for most of the phases.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our website or our YouTube playlist.

TCHEA 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.

In this section:

FCC Medium (MEA) and High Entropy (HEA) Alloys

These examples show some classical calculations of the equilibrium phase stabilities for the FCC medium entropy (MEA) and high entropy (HEA) alloys when using the TCS High Entropy Alloys Database (TCHEA).

CoCrFeNi FCC MEA

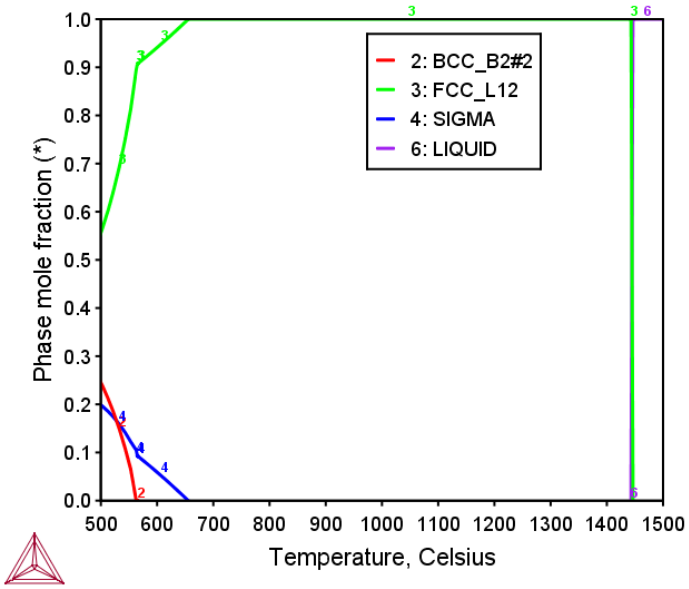

Figure 1: Mole fraction of equilibrium phases at various temperatures in the CoCrFeNi equiatomic alloy [2017Mao].

CoCrFeMnNi FCC HEA

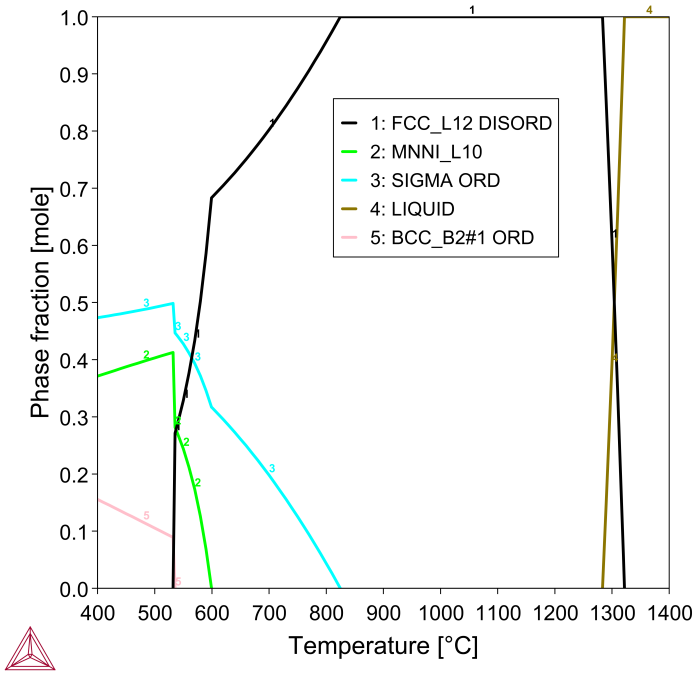

Figure 2: Mole fraction of equilibrium phases at various temperatures in the CoCrFeMnNi equiatomic alloy, a.k.a. the Cantor alloy [2004Can] .

$Co_x(CrFeMnNi)_{100-x}$ FCC HEA

TCS High Entropy Alloys Database (TCHEA) predicts well the melting properties (solidus and liquidus), and stability range of FCC, BCC, sigma, and $L1_0$ phases.

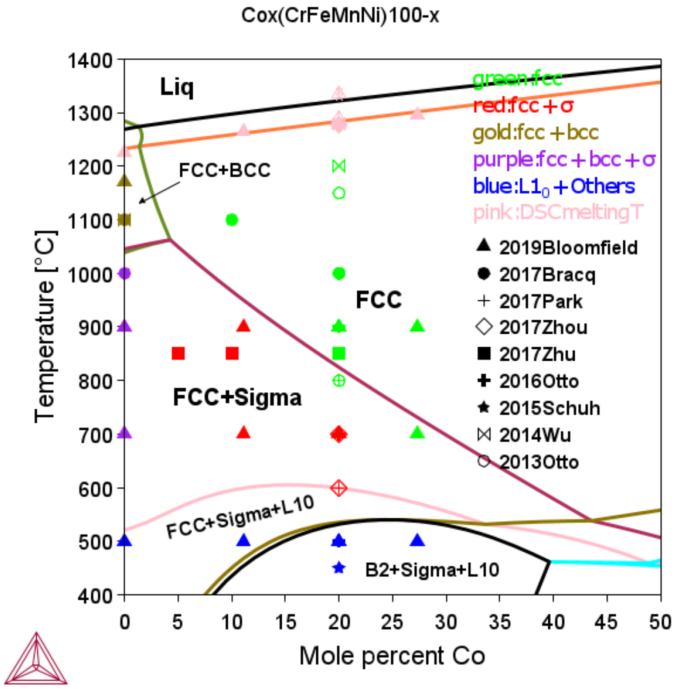

Figure 3: Calculated phase equilibria in the isopleth of Cox(CrFeMnNi)$_{100-x}$, where x represents at% of Co. In the plot, symbols represent experimentally observed phases. These are coded in color for different phase assemblages, e.g. green for single FCC, and red for FCC+Sigma two-phase coexists. Different symbols represent different experimental work. Filled and empty symbols stand for long (>=24 h) and short (<24 h) annealing, respectively.

$CoCrCu_xFeNi$ FCC HEA

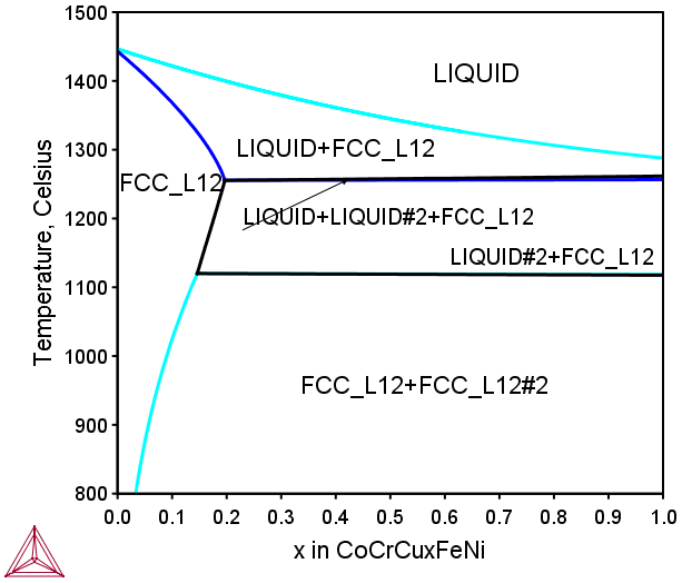

Figure 4: Calculated phase equilibria in the isopleth for the series of the $CoCrCu_xFeNi$ quinary alloys, where x=0-1 represents moles of Cu atoms [2017Mao].

References

[2004Can] B. Cantor, I. T. H. Chang, P. Knight, A. J. B. Vincent, Microstructural development in equiatomic multicomponent alloys. Mater. Sci. Eng. A. 375–377, 213–218 (2004).

[2017Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for “High Entropy” Alloys. J. Phase Equilibria Diffus. 38, 353–368 (2017).

BCC Medium (MEA) and High Entropy (HEA) Alloys

These examples show some classical calculations of the equilibrium phase stabilities for the BCC medium entropy (MEA) and high entropy (HEA) alloys when using the TCS High Entropy Alloys Database (TCHEA).

NbTiVZr BCC MEA

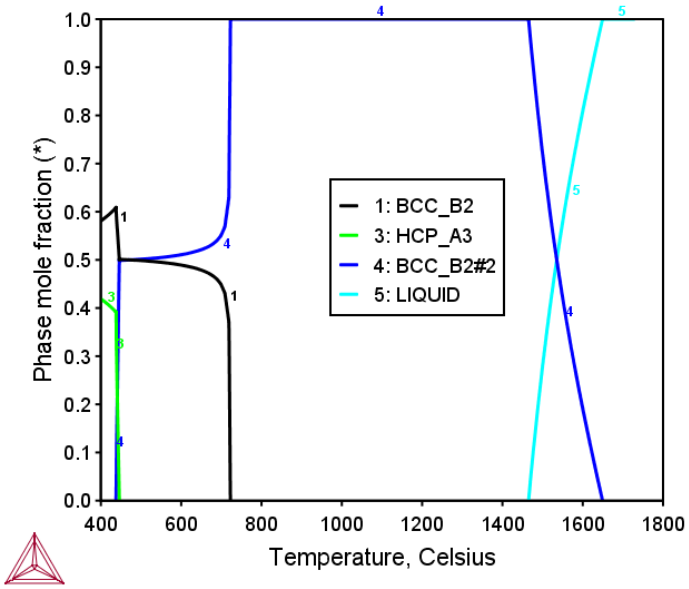

Figure 5: Mole fraction of equilibrium phases at various temperatures in the NbTiVZr equiatomic alloy [2017Mao].

HfNbTaTiZr BCC HEA

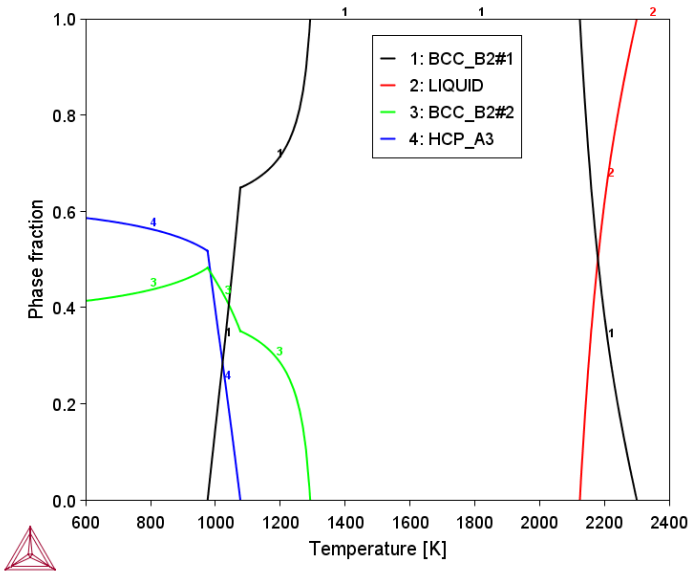

Figure 6: Mole fraction of equilibrium phases at various temperatures in the HfNbTaTiZr equiatomic alloy. The pioneering work of this type of refractory HEA was reported in [2011Sen].

$Al_xNbTaTiV$ BCC HEA

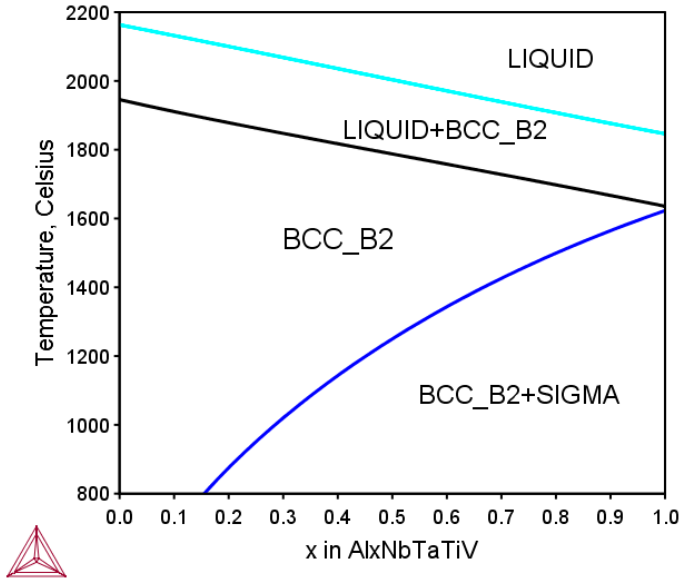

Figure 7: Calculated phase equilibria in the isopleth for the series of the $Al_xNbTaTiV$ quinary alloys, where x=0-1 represents moles of atoms of the element Al [2017Mao].

References

[2011Sen] O. N. Senkov, J. M. Scott, S. V Senkova, D. B. Miracle, C. F. Woodward, Microstructure and room temperature properties of a high-entropy TaNbHfZrTi alloy. J. Alloys Compd. 509, 6043–6048 (2011).

[2017Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for “High Entropy” Alloys. J. Phase Equilibria Diffus. 38, 353–368 (2017).

HCP Medium (MEA) and High Entropy (HEA) Alloys

These examples show some classical calculations of the equilibrium phase stabilities for the HCP medium entropy (MEA) and high entropy (HEA) alloys when using the TCS High Entropy Alloys Database (TCHEA).

CoFeReRu HCP MEA

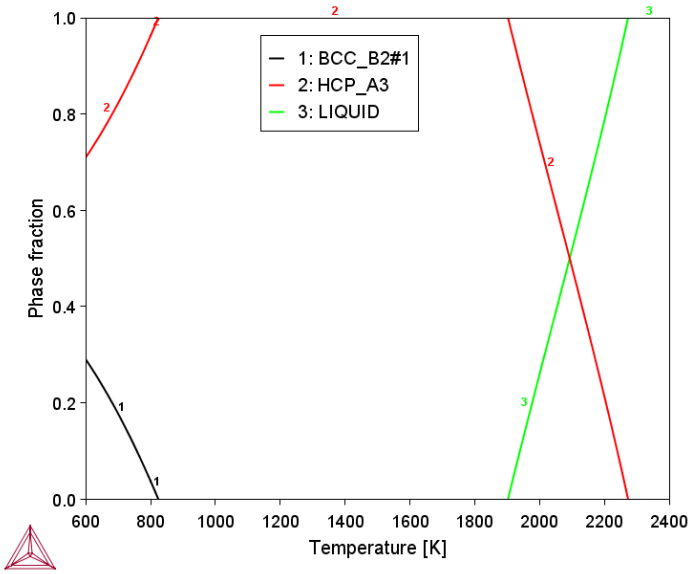

Figure 8: Mole fraction of equilibrium phases at various temperatures in the CoFeReRu equiatomic alloy. The experimental validation is reported in [2016Gao].

IrMoRhRuW HCP HEA

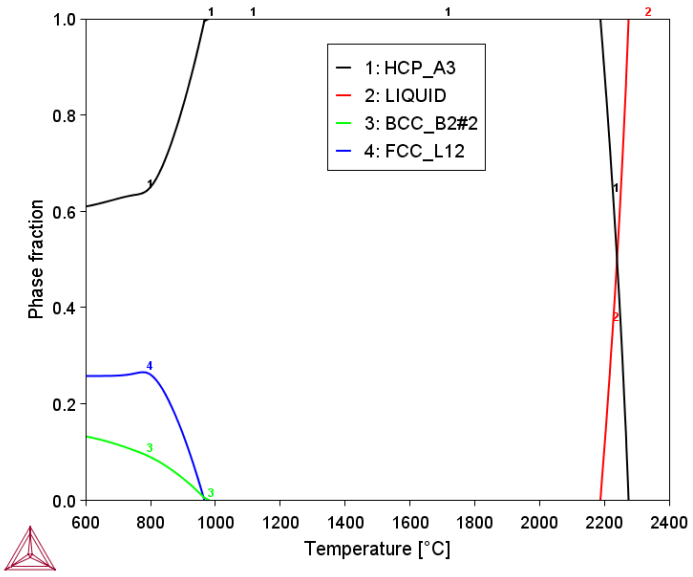

Figure 9: Mole fraction of equilibrium phases at various temperatures in the $Ir_{26}Mo_{20}Rh_{22.5}Ru_{20}W_{11.5}$ high entropy alloy. The experimental validation is reported in [2019Tak].

References

[2016Gao] M. C. Gao, B. Zhang, S. M. Guo, J. W. Qiao, J. A. Hawk, High-Entropy Alloys in Hexagonal Close-Packed Structure. Metall. Mater. Trans. A. 47, 3322–3332 (2016).

[2019Tak] A. Takeuchi, T. Wada, H. Kato, High-Entropy Alloys with Hexagonal Close-Packed Structure in Ir26Mo20Rh22.5Ru20W11.5 and Ir25.5Mo20Rh20Ru25W9.5 Alloys Designed by Sandwich Strategy for the Valence Electron Concentration of Constituent Elements in the Periodic Chart. Mater. Trans. 60, 1666–1673 (2019).

FCC+BCC High Entropy Alloys (HEAs)

These examples show some classical calculations of the equilibrium phase stabilities for the FCC+BCC high entropy (HEA) alloys when using the TCS High Entropy Alloys Database (TCHEA).

$Al_xCoCrFeNi$ FCC+BCC HEAs

This example shows the effect of the Al addition on the phase formation in the equiatomic CoCrFeNi base medium entropy alloy (MEA). The phase formed in as-cast base alloy is dominated by FCC_A1. With a small amount of Al addition (<10 at.% Al), only FCC forms in the as-cast alloys. Adding about 11.11 % Al (x = 0.5) results in the formation of a second phase the B2 phase. The region roughly between 10 and 18 % Al is near the eutectic reaction (eutectic composition 13.98 % Al or x = 0.65), where both FCC and BCC form in as-cast alloys. Further increasing the Al content causes the exchange of the solidification sequence and the primary formation of B2. When the Al content increased up to more than 18.37 at.% Al (x = 0.9), FCC_A1 might be absent during the fast solidification, thus only BCC forms.

The phase formation also depends on the actual experimental conditions, especially the cooling rate and the heat treatment. The data from Wang [2012Wan] indicate the compositions of the investigated as-cast alloys and the observed phases. The data from Kao et al. [2011Kao] are the composition limits for forming BCC, FCC and BCC+FCC in as-cast alloys or alloys homogenized at 1000 °C.

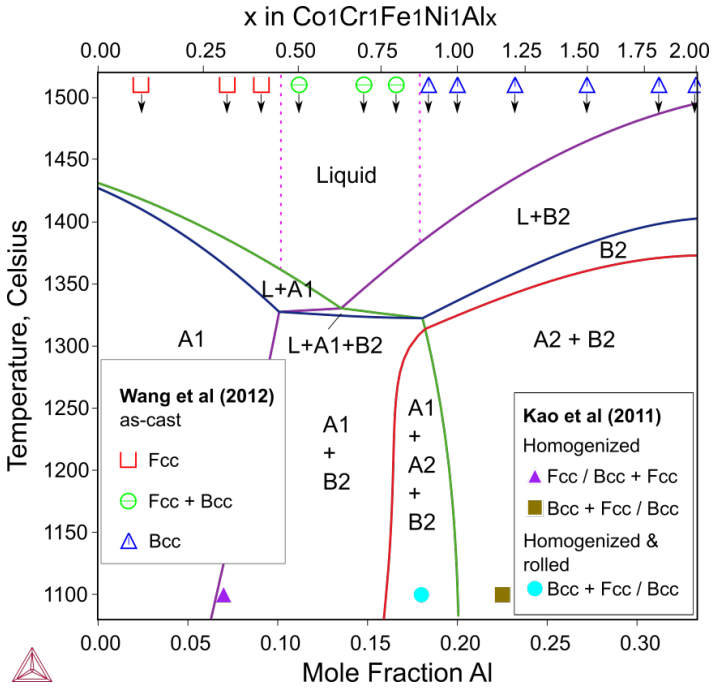

Figure 10: Phase equilibria in the vertical section for $CoCrFeNiAl_x$ (0 < x < 2) alloys [2018Che].

$Al_xCoCrCuFeNi$ FCC+BCC HEAs

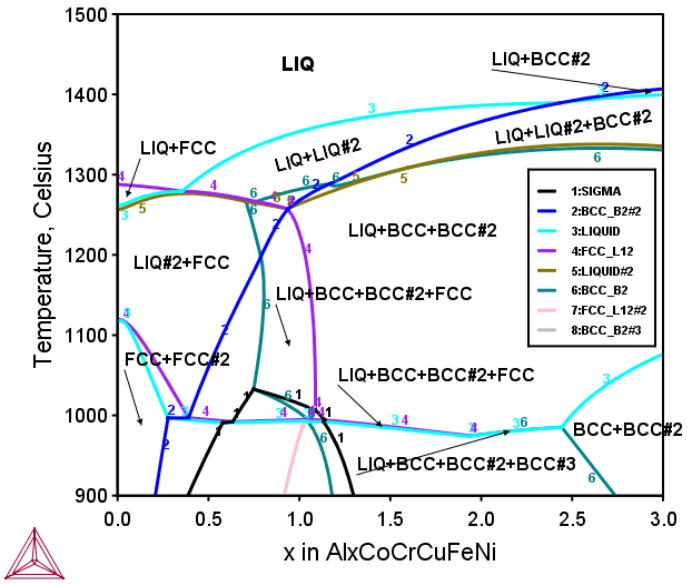

Figure 11: Calculated phase equilibria in the isopleth for the series of the $Al_xCoCrCuFeNi$ senary alloys, where x=0-3 represents moles of atoms of the element Al [2017Mao].

AlCoCrCuFeNiV FCC+BCC HEA

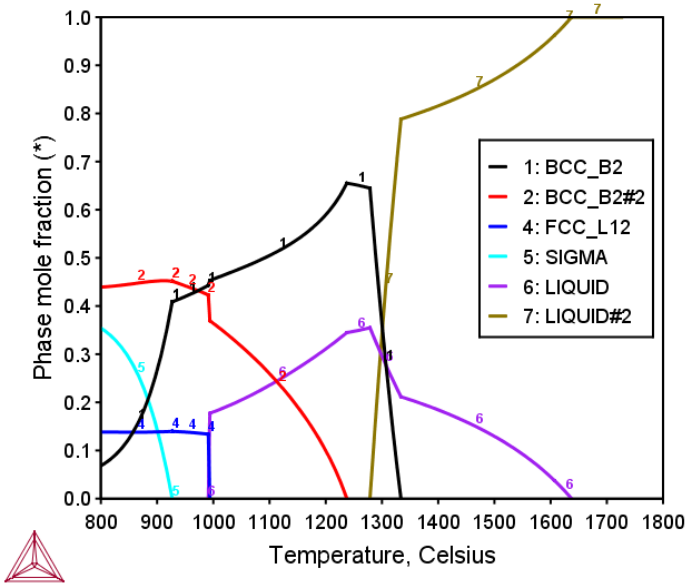

Figure 12: Calculated mole fraction of equilibrium phases at various temperatures in the AlCoCrCuFeNiV septenary alloy with equiatomic ratio [2017Mao].

AlCoCrCuFeNiTiV FCC+BCC HEA

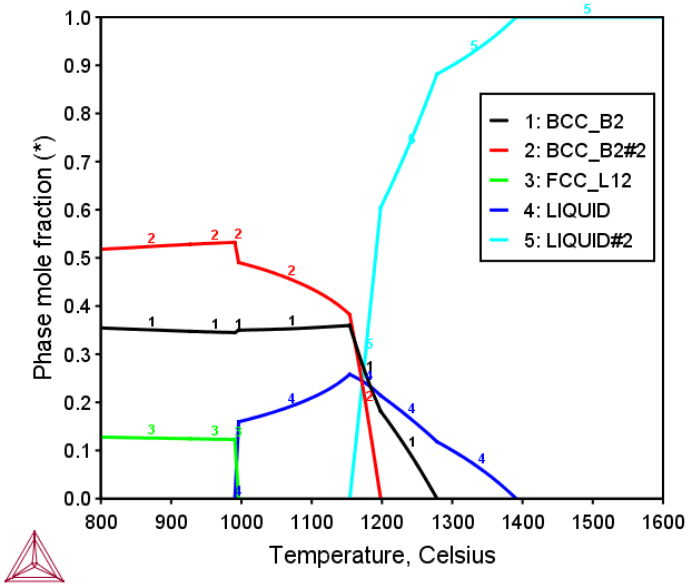

Figure 13: Calculated mole fraction of equilibrium phases at various temperatures in the AlCoCrCuFeNiTiV octonary alloy with equiatomic ratio [2017Mao].

AlCoCrCuFeMnNiTiV FCC+BCC HEA

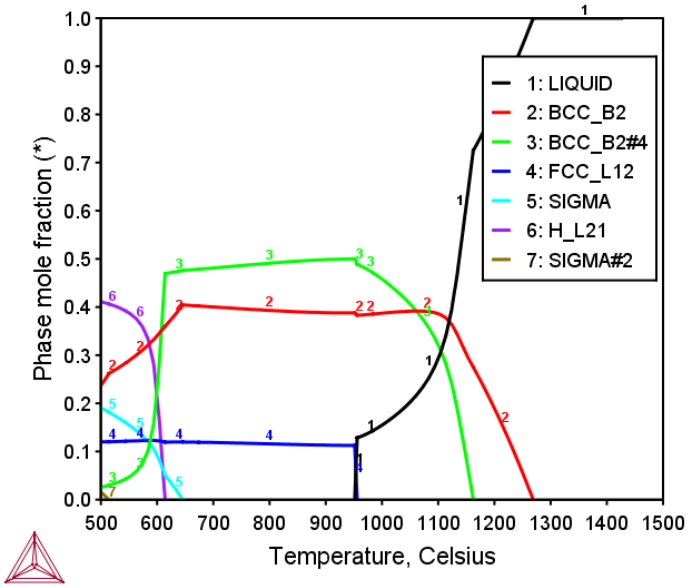

Figure 14: Calculated mole fraction of equilibrium phases at various temperatures in the AlCoCrCuFeMnNiTiV ennead alloy with equiatomic ratio [2017Mao].

References

[2011Kao] Y.-F. Kao, S.-K. Chen, T.-J. Chen, P.-C. Chu, J.-W. Yeh, S.-J. Lin, Electrical, magnetic, and Hall properties of AlxCoCrFeNi high-entropy alloys. J. Alloys Compd. 509, 1607–1614 (2011).

[2012Wan] W.-R. Wang, W.-L. Wang, S.-C. Wang, Y.-C. Tsai, C.-H. Lai, J.-W. Yeh, Effects of Al addition on the microstructure and mechanical property of AlxCoCrFeNi high-entropy alloys. Intermetallics. 26, 44–51 (2012).

[2017Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for “High Entropy” Alloys. J. Phase Equilibria Diffus. 38, 353–368 (2017).

[2018Che] H.-L. Chen, H. Mao, Q. Chen, Database development and Calphad calculations for high entropy alloys: Challenges, strategies, and tips. Mater. Chem. Phys. 210, 279–290 (2018).

Oxidation Behaviors in High Entropy Alloys

These examples show the application of oxidation when using the TCS High Entropy Alloys Database (TCHEA). Including oxygen (O) in the simulations allows for the study of oxidation behaviors of HEAs at various compositions, temperatures, and oxygen activities.

The element oxygen (O) and relevant oxide phases are included in the database starting with version 8.0 (TCHEA8).

Oxidation of $Al_xCoCrFeNi$

This is an example of the oxidation of $Al_xCoCrFeNi$ HEAs at 1273 K. The plot shows that with the increase of Al, the microstructure of the base HEA Al_x(CoCrFeNi) shifts from a single FCC to dual B2+FCC, where the inner oxidation product corundum shifts from Cr_2O_3- to Al_2O_3-dominant.

At high Al, for example 9 and 12 at%, Al_2O_3 corundum is stable at very low oxygen activity. There is various multicomponent spinel phases that result as inner oxidation products. When Al is increased, the spinel phase contains more Cr but less Fe. Also, halite forms at low Al alloys. Overall, it predicts improved oxidation-resistance with the increase of Al, which agrees well with the experimental observation of [2021Dab].

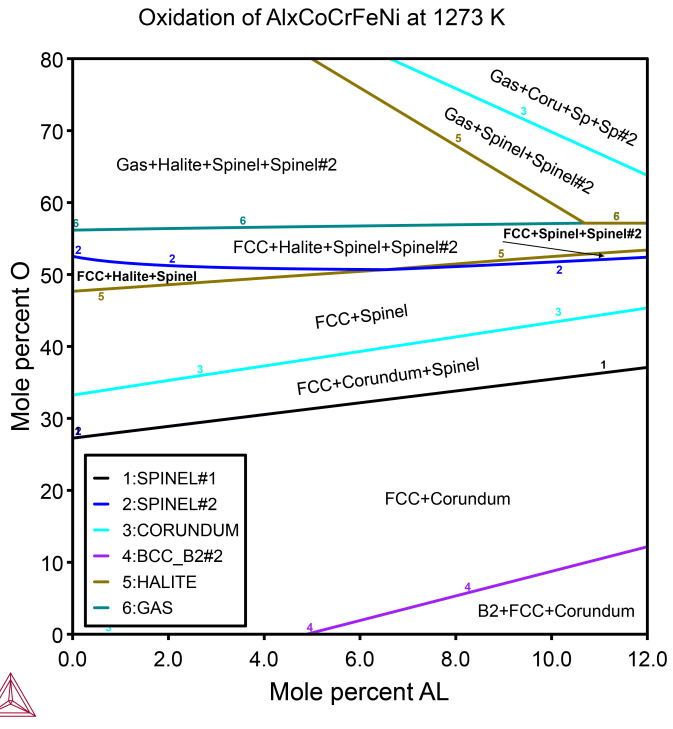

Figure 15: The oxidation of $Al_xCoCrFeNi$ HEAs at 1273 K.

Oxidation Resistant Refractory HEA Protected by Rutile Oxide

The microstructure of the alloy Al17.6Cr25.2Mo20.3Nb15.2Si2.9Ta13.4Ti5.4 (at%) consists of three phases (BCC + Sigma + Laves). The main oxidation products are rutile ($CrTaO_4$ dissolving Al, Cr, Ti, etc.) and corundum (Al_2O_3 and Cr_2O_3). The MoO_3-dominant liquid around x(O)=0.7 indicates the porous oxide scale. Most important, the continuous rutile oxide scale attributes to the high oxidation-resistance of this RHEA, which agrees well with the experimental observation of Lo et al. [2019Lo].

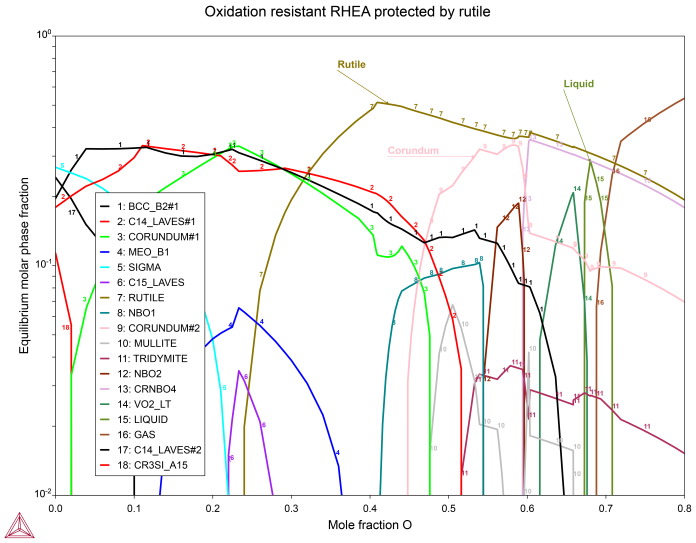

Figure 16: An example of the oxidation resistant refractory HEA alloy Al17.6Cr25.2Mo20.3Nb15.2Si2.9Ta13.4Ti5.4 (at%) with the main oxidation products of rutile and corundum.

References

[2019Lo] K.-C. Lo, Y.-J. Chang, H. Murakami, J.-W. Yeh, A.-C. Yeh, An oxidation resistant refractory high entropy alloy protected by CrTaO4-based oxide. Sci. Rep. 9, 7266 (2019).

[2021Dab] J. Dąbrowa, G. Cieślak, M. Stygar, M. Zajusz, M. Jawańska, A. Gil, J. Jedliński, K. Mroczka, K. Matsuda, T. Kulik, M. Danielewski, Oxidation Behavior of Alx(CoCrFeNi)100-x High-Entropy Alloys Under Thermal-Cycling Conditions. Oxid. Met. 96, 307–321 (2021).

Molar Volume and Density

The TCS High Entropy Alloys Database (TCHEA) includes molar volume information for all phases, which allows calculation of volume, thermal expansion, and density vs. composition and temperature. It can be used for design, and as inputs to other codes e.g. the finite element method (FEM).

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.

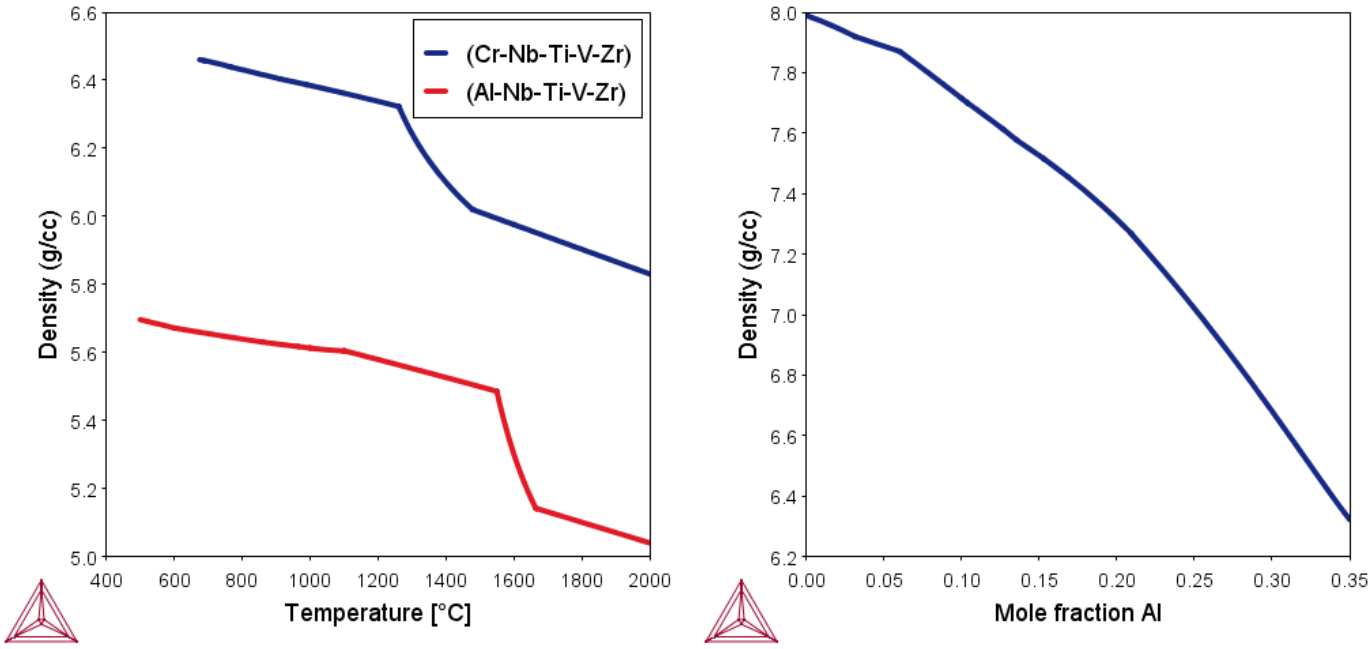

Figure 17: Calculated density of HEAs. (a) Density of CrNbTiVZr and AlNbTiVZr HEAs at various temperatures. The measured room temperature density is 6.57 g/cc for CrNbTiVZr [2013Sen] and 5.79 g/cc for AlNbTiVZr [2015Ste]. (b) Density of AlxCoCrFeNi HEAs at 400°C.

The following table shows the experimental and calculated densities of some BCC HEAs.

As-cast HEAs	*HfNbTaTiZr*	*MoNbTaVW*	*MoNbTaW*	*AlCrTiV*
Phase Exp (Calc)	BCC (BCC)	BCC (BCC)	BCC (BCC)	B2 (B2)
Density, g/cm^3 Exp (Calc)	9.94 (9.92)	12.36 (12.35)	13.75 (13.80)	5.06 (5.04)

As-cast HEAs	HfNbTaTiZr	MoNbTaVW	MoNbTaW	AlCrTiV
Experimental reference	[2011Sen]	[2010Sen]	[2010Sen]	[2017Qiu]

The following table shows the calculated lattice parameter and density compared to experimental data. Calculation was made at 673K with experimental data from [2018Lap].

	LP Exp. (nm)	LP Cal. (nm)	Density Exp. (g/cm^3	Density Cal. (g/cm^3)
CrFeCoNi	0.357	0.359	8.1	8.03
CrCoNi	0.357	0.359	8.2	8.08
CrFeNi	0.359	0.360	7.9	7.88
FeCoNi	0.358	0.359	8.4	8.30
MnCoNi	0.360	0.363	8.1	7.91
MnFeNi	0.362	0.365	7.9	7.81
CoNi	0.354	0.356	8.8	8.62

References

[2010Sen] O. N. Senkov, G. B. Wilks, D. B. Miracle, C. P. Chuang, P. K. Liaw, Refractory high-entropy alloys. Intermetallics. 18, 1758–1765 (2010).

[2011Sen] O. N. Senkov, J. M. Scott, S. V Senkova, D. B. Miracle, C. F. Woodward, Microstructure and room temperature properties of a high-entropy TaNbHfZrTi alloy. J. Alloys Compd. 509, 6043–6048 (2011).

[2013Sen] O. N. Senkov, S. V Senkova, D. B. Miracle, C. Woodward, Mechanical properties of low-density, refractory multi-principal element alloys of the Cr–Nb–Ti–V–Zr system. Mater. Sci. Eng. A. 565, 51–62 (2013).

[2015Ste] N. D. Stepanov, N. Y. Yurchenko, D. G. Shaysultanov, G. A. Salishchev, M. A. Tikhonovsky, Effect of Al on structure and mechanical properties of Al x NbTiVZr (x = 0, 0.5, 1, 1.5) high entropy alloys. Mater. Sci. Technol. 31, 1184–1193 (2015).

[2017Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for “High Entropy” Alloys. J. Phase Equilibria Diffus. 38, 353–368 (2017).

[2017Qiu] Y. Qiu, Y. J. Hu, A. Taylor, M. J. Styles, R. K. W. Marceau, A. V. Ceguerra, M. A. Gibson, Z. K. Liu, H. L. Fraser, N. Birbilis, A lightweight single-phase AlTiVCr compositionally complex alloy. Acta Mater. 123, 115–124 (2017).

[2018Lap] 1. G. Laplanche, P. Gadaud, C. Bärsch, K. Demtröder, C. Reinhart, J. Schreuer, E. P. George, Elastic moduli and thermal expansion coefficients of medium-entropy subsystems of the CrMnFeCoNi high-entropy alloy. J. Alloys Compd. 746, 244–255 (2018).

Thermal Conductivity

Thermal Conductivity (THCD) of HEAs can be calculated using Thermo-Calc and with the TCS High Entropy Alloys Database (TCHEA). You can calculate the quantities of a phase ϕ such as FCC or BCC with the variables THCD(ϕ), or a system (i.e. alloy) with barely 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 (THCD) starting with version 5.0 (TCHEA5).

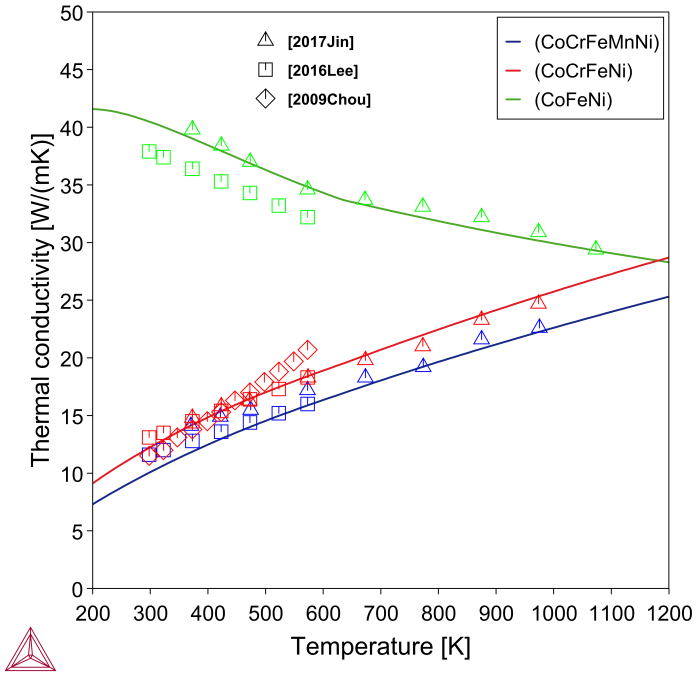

Figure 18: Thermal conductivity of equiatomic FCC medium- and high-entropy alloys at various temperatures. Curves represent calculations while symbols for experimental data from different literature. Each alloy (composition) is assigned a specific color.

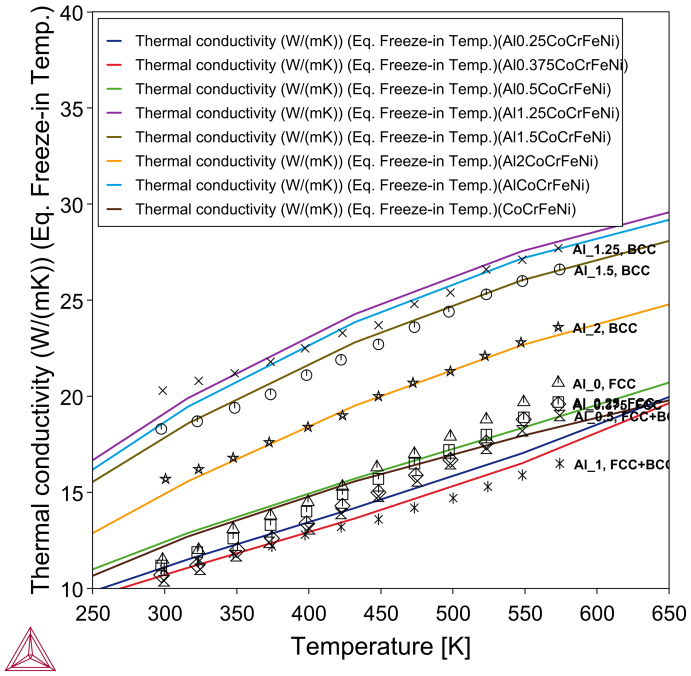

Figure 19: Thermal conductivity of $Al_xCoCrFeNi$ high-entropy alloys at various temperatures. Curves represent (freeze-in) calculations while symbols for experimental data (of as-homogenized alloys at 1373 K) from the literature [2009Chou]. The notation e.g. "Al_1.25, BCC" implies the experimental series for the alloy $Al_{1.25}CoCrFeNi$ with BCC structure.

References

[2009Chou] H.-P. Chou, Y.-S. Chang, S.-K. Chen, J.-W. Yeh, Microstructure, thermophysical and electrical properties in AlxCoCrFeNi (0≤x≤2) high-entropy alloys. Mater. Sci. Eng. B. 163, 184–189 (2009).

[2016Lee] J. I. Lee, H. S. Oh, E. S. Park, Manipulation of σ y /κ ratio in single phase FCC solid-solutions. Appl. Phys. Lett. 109, 061906 (2016).

[2017Jin] K. Jin, S. Mu, K. An, W. D. Porter, G. D. Samolyuk, G. M. Stocks, H. Bei, Thermophysical properties of Ni-containing single-phase concentrated solid solution alloys. Mater. Des. 117, 185–192 (2017).

Electrical Resistivity

Electrical resistivity (ELRS) of HEAs can be calculated using Thermo-Calc and with the TCS High Entropy Alloys Database (TCHEA). You can calculate the quantities of a phase ϕ such as FCC or BCC with the variables ELRS(ϕ), or a system (i.e. alloy) with ELRS. You can also calculate the derived quantities, i.e. electrical conductivity (ELCD) in a similar way.

The database includes electrical resistivity (ELRS) starting with version 5.0 (TCHEA5).

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.

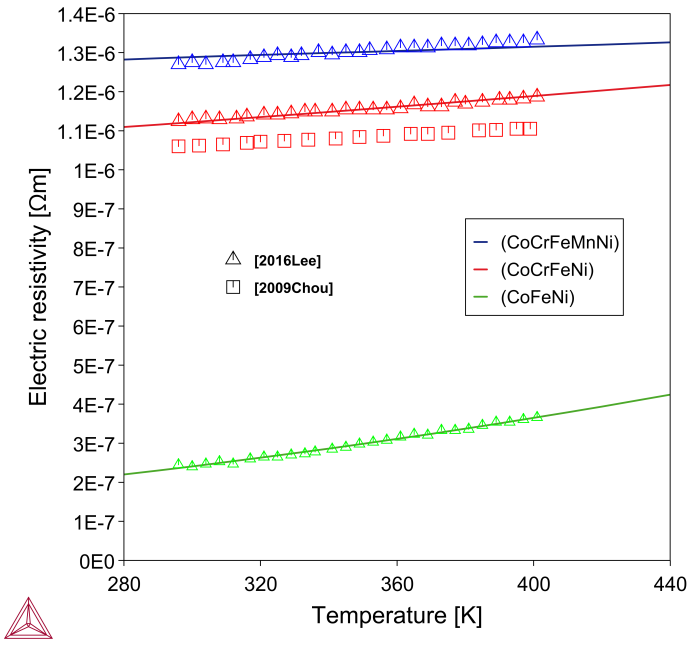

Figure 20: Electrical resistivity of equiatomic FCC medium- and high-entropy alloys at various temperatures. Curves represent calculations while symbols for experimental data from different literature. Each alloy (composition) is assigned a specific color.

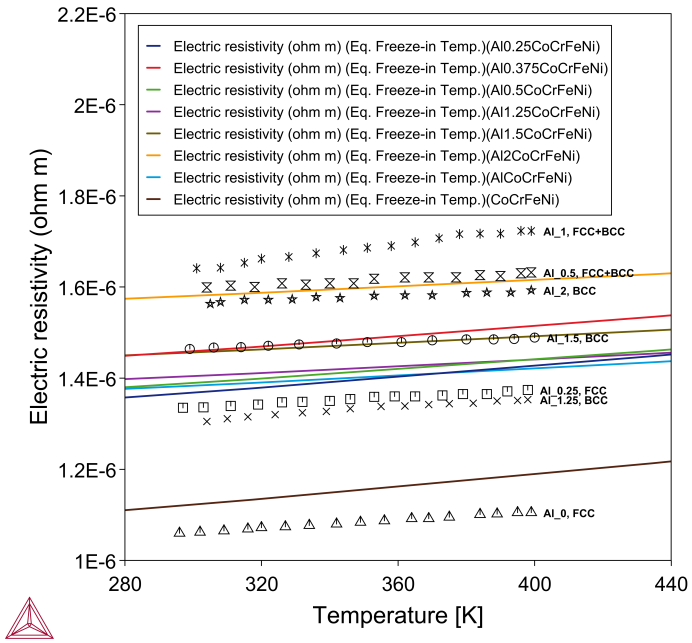

Figure 21: Electrical resistivity of $Al_xCoCrFeNi$ high-entropy alloys at various temperatures. Curves represent (freeze-in) calculations while symbols for experimental data (of as-homogenized alloys at 1373 K) from the literature [2009Chou]. The notation e.g. "Al_0.375, FCC" implies the experimental data for the alloy $Al_{0.375}CoCrFeNi$ with single FCC phase.

References

[2009Chou] H.-P. Chou, Y.-S. Chang, S.-K. Chen, J.-W. Yeh, Microstructure, thermophysical and electrical properties in AlxCoCrFeNi (0≤x≤2) high-entropy alloys. Mater. Sci. Eng. B. 163, 184–189 (2009).

[2016Lee] J. I. Lee, H. S. Oh, E. S. Park, Manipulation of σ y /κ ratio in single phase FCC solid-solutions. Appl. Phys. Lett. 109, 061906 (2016).

[2017Jin] K. Jin, S. Mu, K. An, W. D. Porter, G. D. Samolyuk, G. M. Stocks, H. Bei, Thermophysical properties of Ni-containing single-phase concentrated solid solution alloys. Mater. Des. 117, 185–192 (2017).

Viscosity of Cu-Ni-Al-Co-Fe Alloy

Viscosity of liquid can be calculated directly using the TCS High Entropy Alloys Database (TCHEA) as a function of chemical composition and temperature.

The viscosity thermophysical property data is included with the TCS High Entropy Alloys Database (TCHEA) starting with version 4 (TCHEA4).

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 kinematic viscosity of equiatomic liquid alloy Cu-Ni-Al-Co-Fe is shown.

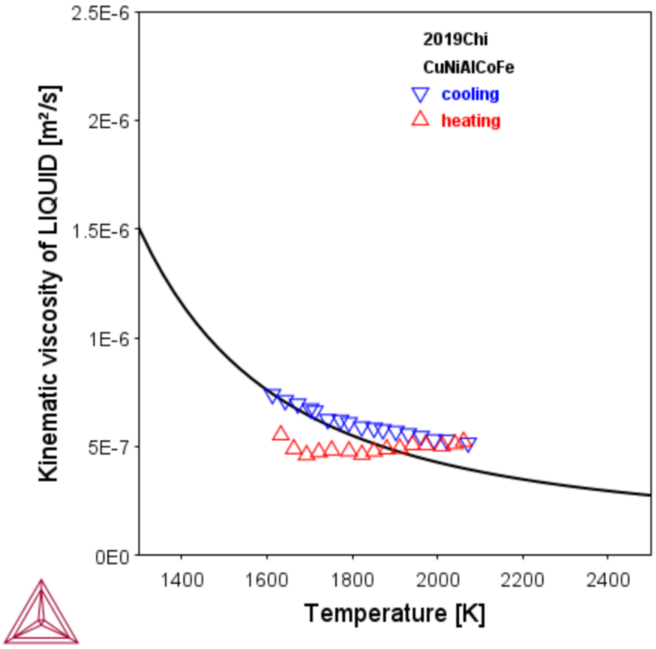

Figure 22: Calculated kinematic viscosity of equiatomic Cu-Ni-Al-Co-Fe alloy along with experimental data from [2019Chi].

Reference

[2019Chi] O. Chikova, V. Tsepelev, V. V'yukhin, K. Shmakova, V. Il'in, Viscosity and Electrical Resistivity of Liquid CuNiAl, CuNiAlCo, CuNiAlCoFe Alloys of Equiatomic Compositions. Acta Metall. Slovaca. 25, 259–266 (2019).

Surface Tension of Cu-Fe-Ni

The surface tension thermophysical property data is included with the TCS High Entropy Alloys Database (TCHEA) starting with version 5 (TCHEA5).

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.

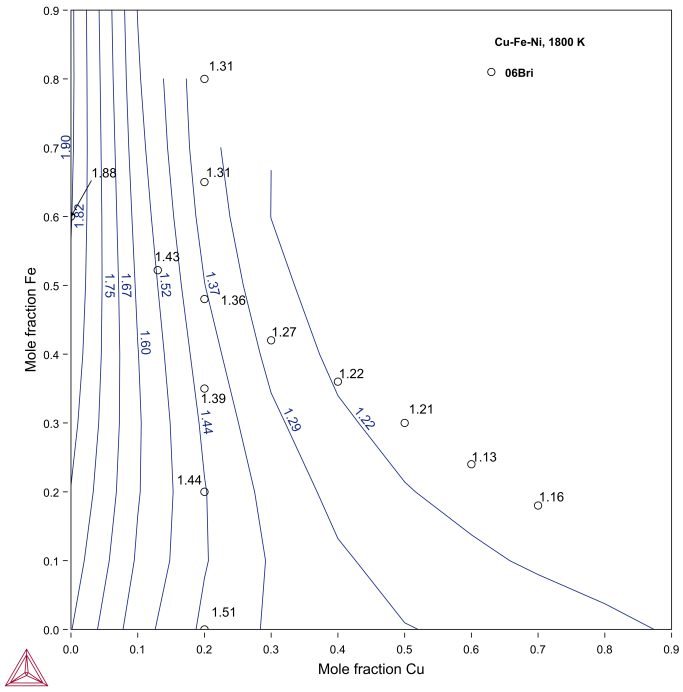

Figure 23: Calculated surface tension of ternary Cu-Fe-Ni liquid at 1800 K in comparison with experimental data of [2006Bri].

Reference

[2006Bri] J. Brillo, I. Egry, T. Matsushita, Density and Surface Tension of Liquid Ternary Ni–Cu–Fe Alloys. Int. J. Thermophys. 27, 1778–1791 (2006).

Yield Strength

In Thermo-Calc, a Yield Strength Model is available with the Property Model Calculator and directly calculates yield stress. Yield strength is also available as a variable when working with Plots and Tables that are successors to the Precipitation Calculator. When using the Add-on Precipitation Module (TC-PRISMA), the Yield Strength Model returns the yield strength at room temperature for the specified material using the equilibrium values calculated at temperature *T*. The Model is defined by further setting the following contributions: intrinsic strength, solid solution strengthening, grain boundary strengthening and precipitation strengthening.

Read more on our website about Property Models, including information about the material specific Model Libraries (i.e steel, nickel, titanium, etc.), 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.

Mo-Ta BCC Binary Alloy

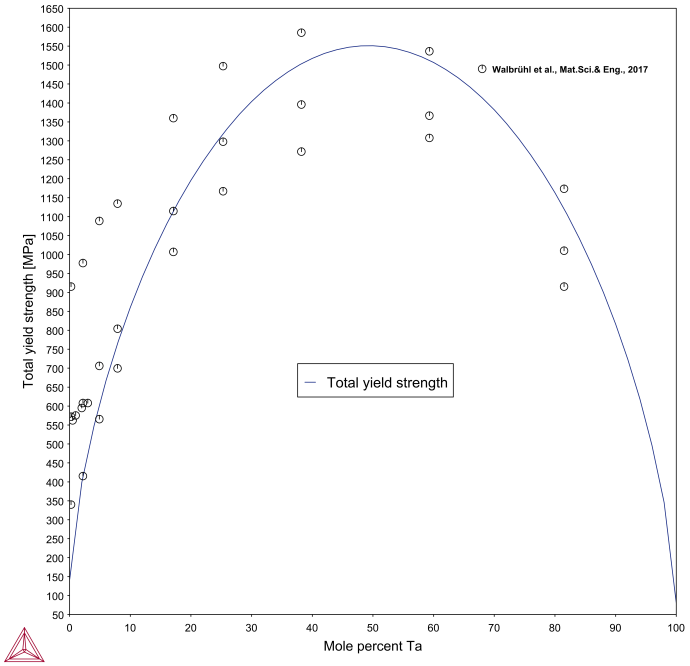

Figure 24: Total yield strength of the Mo-Ta BCC binary alloy in comparison with the experimental data from [2017Wal]. This example is included with Thermo-Calc as a Property Model example named PM_G_06_Yield_Strength_HEA.

Reference

[2017Wal] M. Walbruhl, D. Linder, J. Ågren, A. Borgenstam, Modelling of solid solution strengthening in multicomponent alloys. Mater. Sci. Eng. A. 700, 301–311 (2017).

Elastic Constants in a Cantor Alloy

The TCS High Entropy Alloys Database (TCHEA) has elastic properties included starting with version 8 (TCHEA8).

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 application example shows where the elastic constants are calculated as a function of temperature for a single-phase FCC_A1 and near-equiatomic CoCrFeMnNi alloy, commonly referred to as a Cantor alloy.

In the calculation setup, the composition Co21.1Cr20.9Fe19.7Mn16.7Ni21.6 (at. %) is used, which is experimentally measured by [2019Ter]. The resulting values of the elastic constants are in good agreement with the experimental data from [2019Ter; 2021Kaw].

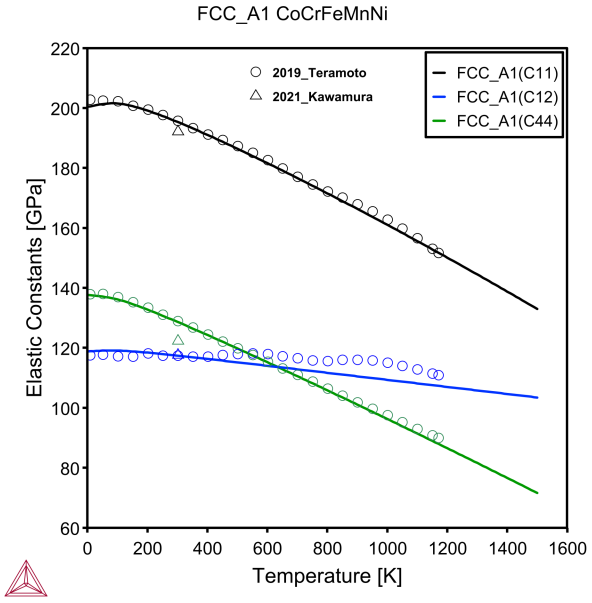

Figure 25: Elastic constants of the FCC_A1 Cantor alloy Co21.1Cr20.9Fe19.7Mn16.7Ni21.6 (at. %) as a function of temperature compared to experimental data from [2019Ter; 2021Kaw].

References

[2019Ter] T. Teramoto, K. Yamada, R. Ito, K. Tanaka, Monocrystalline elastic constants and their temperature dependences for equi-atomic Cr-Mn-Fe-Co-Ni high-entropy alloy with the face-centered cubic structure. J. Alloys Compd. 777, 1313–1318 (2019).

[2021Kaw] M. Kawamura, M. Asakura, N. L. Okamoto, K. Kishida, H. Inui, E. P. George, Plastic deformation of single crystals of the equiatomic Cr−Mn−Fe−Co−Ni high-entropy alloy in tension and compression from 10 K to 1273 K. Acta Mater. 203, 116454 (2021).

Solidification Simulation (Equilibrium vs Scheil)

Equilibrium and Scheil simulations can be used to study the solidification microstructure evolution. Calculated fractions and compositions of solid and liquid phases help understand the segregation profile and guide homogenization temperatures/time.

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.

$CoCrFeNiAl_{1.1}$ Alloy

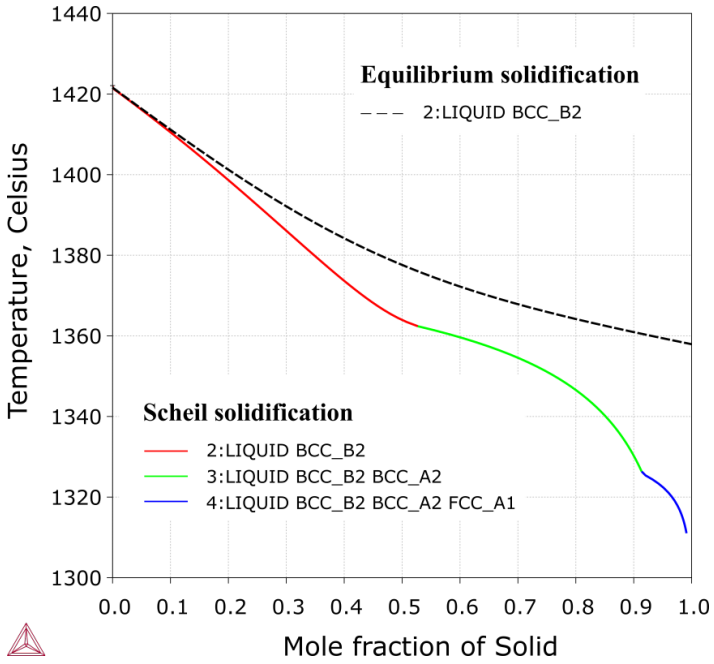

Figure 26: Equilibrium (in dashed line) and Scheil (in solid line) solidification simulations of the $CoCrFeNiAl_{1.1}$ alloy (21.57 at.% Al) [2018Che].

$CoCrFeNiZr_{0.4}$ Alloy

Scheil simulations are helpful to understand the solidification behavior during fast cooling. In the as-cast CoCrFeNiZr0.4 alloy, in addition to the FCC and C15_Laves phase, a minor amount of Ni7Zr2 phase was observed [2017She]. According to the equilibrium calculation, and shown by the black curves in Figure 27, no Ni7Zr2 phase was predicted. However, the Scheil simulation, the red curves in the same figure, does predicts a minor fraction of solidification of Ni7Zr2. You can consider that the global equilibrium calculation and the Scheil simulation mimic two extreme conditions for the solidification process. A real case should happen at the condition in between, depending on the kinetic conditions.

Starting with Thermo-Calc version 2020a, it is also possible to take the back-diffusion into account using the Scheil Calculator in Graphical Mode.

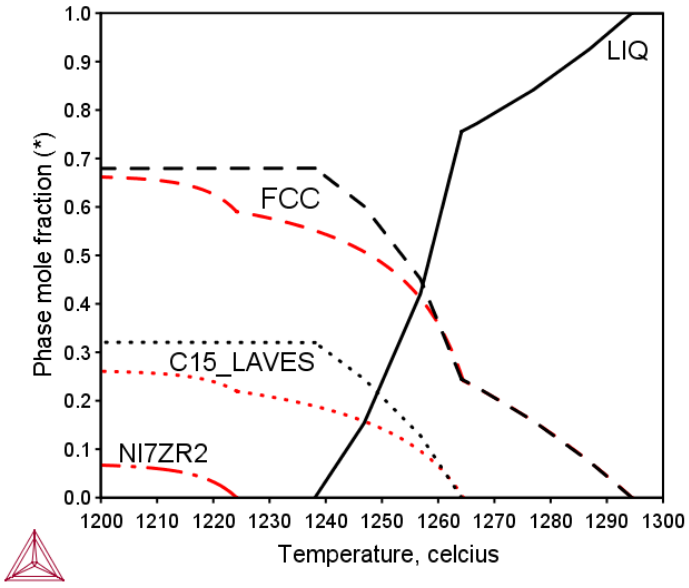

Figure 27: Predicted solid phase mole fractions by equilibrium (black curves) and Scheil simulation (red curves) of the CoCrFeNiZr0.4 alloy [2017Mao].

$CoCrFeNiAl_{0.65}$ Alloy

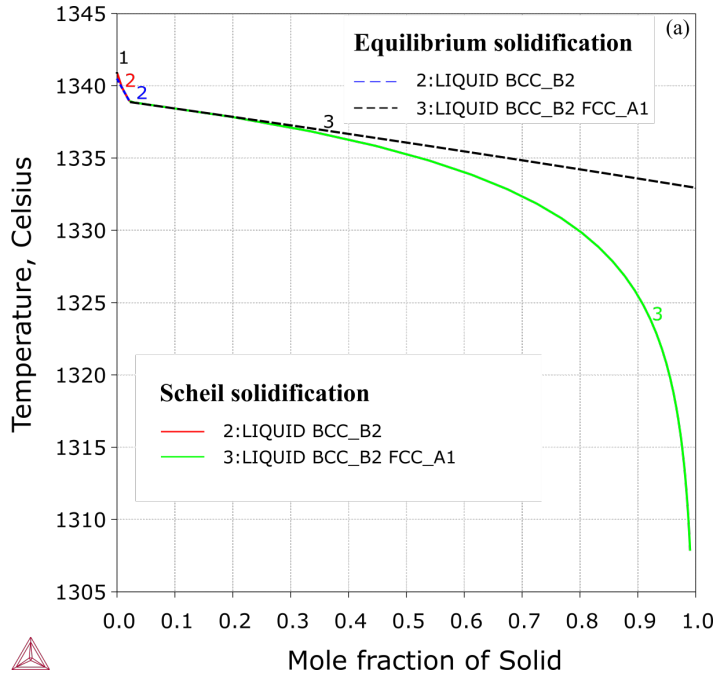

Figure 28: Solidification simulation of the eutectic alloy $CoCrFeNiAl_{0.65}$ (13.98 at.% Al): Phase formation sequence and solid phase fractions from equilibrium (in dashed line) and Scheil simulation (solid line) [2018Che].

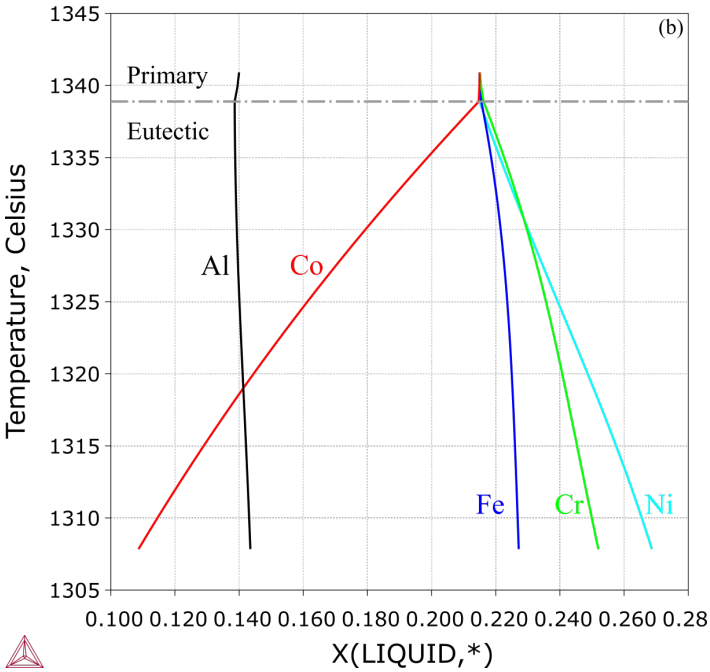

Figure 29: Solidification simulation of the eutectic alloy $CoCrFeNiAl_{0.65}$ (13.98 at.% Al): Liquid phase composition from a Scheil simulation [2018Che].

CoCrCuFeMnNi Alloy

The solidification of the CoCrCuFeMnNi alloy starts with the formation of a Cu-lean FCC_A1 phase, corresponding to the dendrites observed in the as-cast alloy [2004Can]. The second FCC_A1 phase (labeled as FCC_A1#2 in Figure 30), which is Cu-rich starts to form when only about 30% liquid remains. Among the minor alloying elements, Mn and Ni have noticeably higher contents than Co, Cr and Fe. The equilibrium solidification ends at the concurrent formation of the two FCC phases, while the Scheil simulation even predicts the formation of a Cr-rich BCC_A2. No BCC_A2 phase was reported, which probably attributes either its amount was too little to be detected with XRD, or its formation was suspended by the rapid cooling.

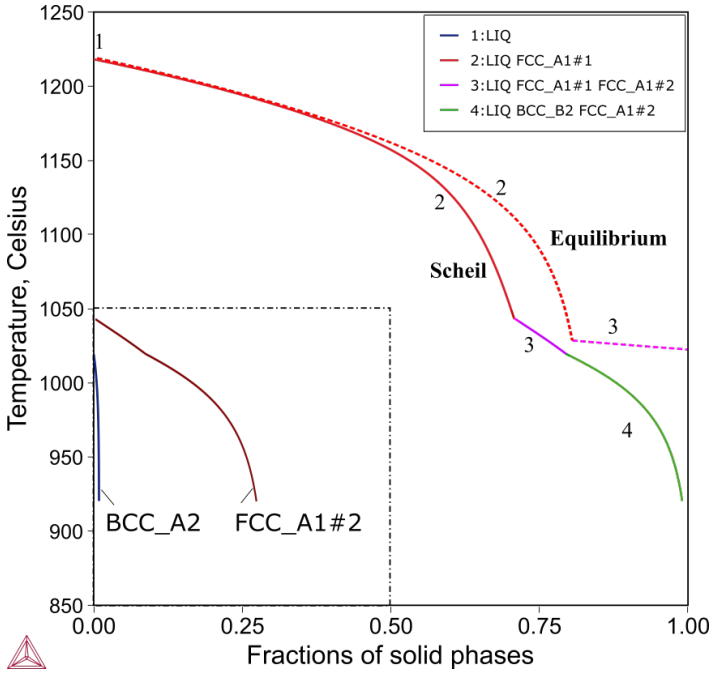

Figure 30: Scheil and equilibrium calculations of the CoCrCuFeMnNi alloy. Total and individual solid phase fraction from the Scheil simulation (in solid lines) and equilibrium calculation (in dashed lines) of CoCrCuFeMnNi. The phase fractions of the minor phases (FCC_A1#2 and BCC_A2) are imposed and enclosed with the dashed-dotted lines.

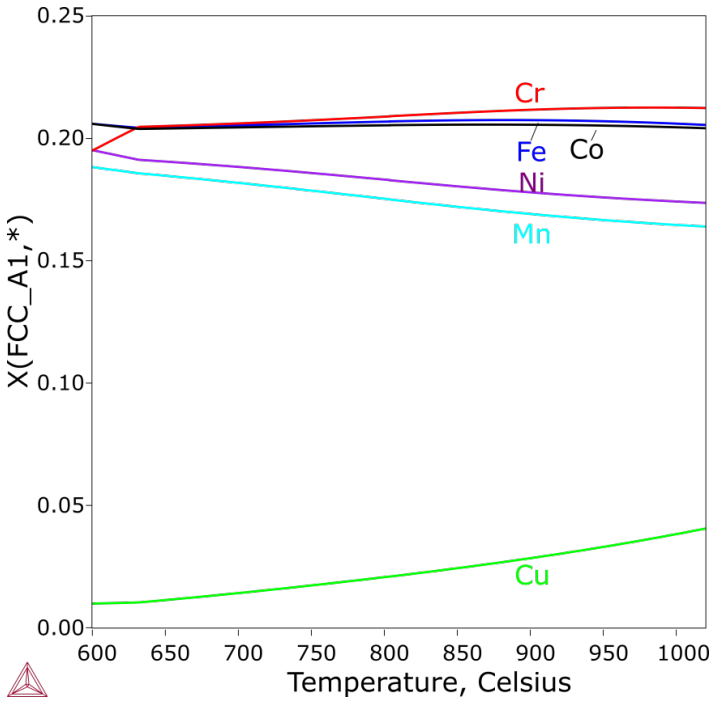

Figure 31: Scheil calculation of the CoCrCuFeMnNi alloy. The composition of the Cu-lean FCC_A1 dendritic phase from the Scheil simulation of CoCrCuFeMnNi.

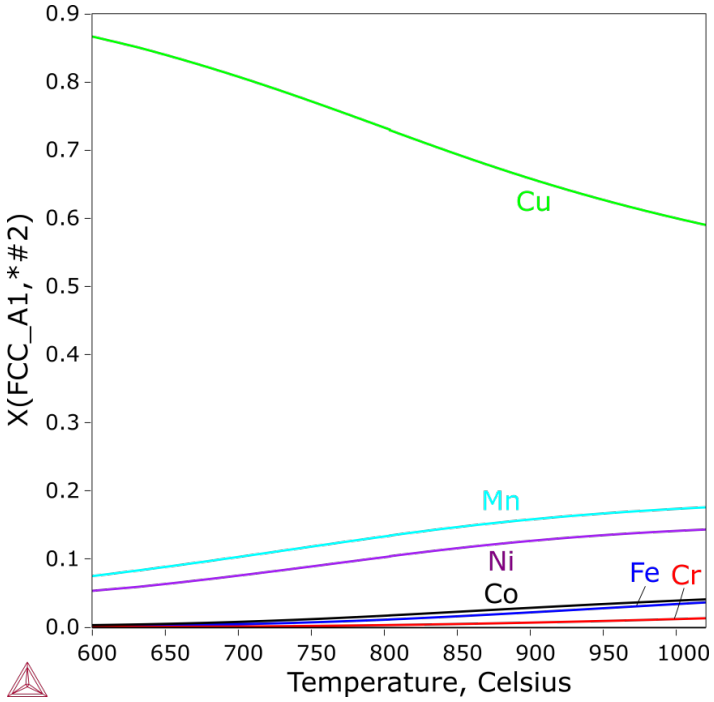

Figure 32: Scheil calculation of the CoCrCuFeMnNi alloy. The composition of the Cu-rich FCC_A1 interdendritic phase from the Scheil simulation of CoCrCuFeMnNi.

References

[2004Can] B. Cantor, I. T. H. Chang, P. Knight, A. J. B. Vincent, Microstructural development in equiatomic multicomponent alloys. Mater. Sci. Eng. A. 375–377, 213–218 (2004).

[2017Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for “High Entropy” Alloys. J. Phase Equilibria Diffus. 38, 353–368 (2017).

[2017She] S. Sheikh, H. Mao, S. Guo, Predicting solid solubility in CoCrFeNiM x (M = 4d transition metal) high-entropy alloys. J. Appl. Phys. 121, 194903 (2017).

[2018Che] H.-L. Chen, H. Mao, Q. Chen, Database development and Calphad calculations for high entropy alloys: Challenges, strategies, and tips. Mater. Chem. Phys. 210, 279–290 (2018).

Diffusion Simulations (DICTRA)

Combining the TCS High Entropy Alloys Database (TCHEA) with its compatible TCS High Entropy Alloy Mobility Database (MOBHEA), the elemental diffusion and diffusion control phase transformation can be simulated using the Diffusion Calculator, which is part of the Add-on Diffusion Module (DICTRA) in Thermo-Calc.

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.

Interdiffusion of FCC HEAs

This example shows the simulation of interdiffusion in the diffusion couple of two FCC HEAs namely Co30Cr20Fe25Ni10Mn15 and Co10Cr20Fe15Ni30Mn25 (at %) in comparison with experimental information from [2017Ver].

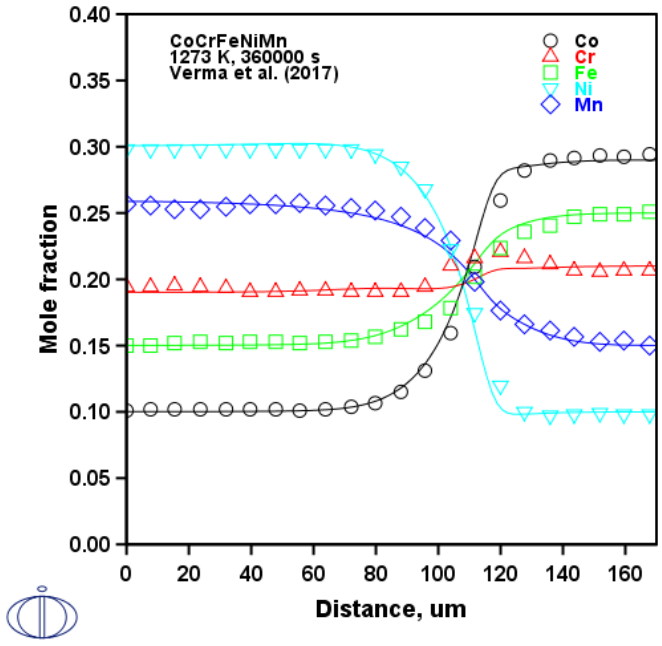

Figure 33: A Diffusion Module (DICTRA) simulated concentration profile of FCC HEA diffusion couple annealed at 1000 °C for 100 hours. Experimental data from [2017Ver].

Interdiffusion of BCC HEAs

In this example, the simulations were performed at a temperature of 1373 K annealed after 64800 s, where the composition of the diffusion couple is Ti-0.222Nb-0.078Ta/Ti-0.144Nb-0.069Ta-0.058Zr (unit: mole fraction) with a BCC_A2 phase.

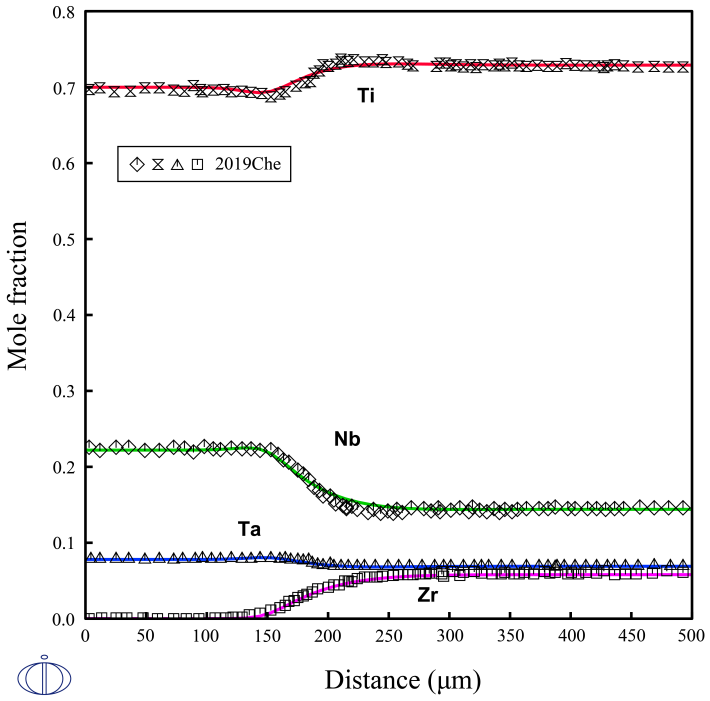

Figure 34: Simulated concentration profiles of diffusion couple Ti-0.222Nb-0.078Ta/Ti-0.144Nb-0.069Ta-0.058Zr with BCC_A2 phase annealed after 64800 s at 1373 K compared with the experimental data [2019Che].

Kinetics of Fe/Ti Diffusion Couples

The simulations were performed using the homogenization model available with the Diffusion Module (DICTRA). The concentration profiles of Fe in the diffusion couple Fe/Ti at a temperature of 1273 K are annealed after 1 h.

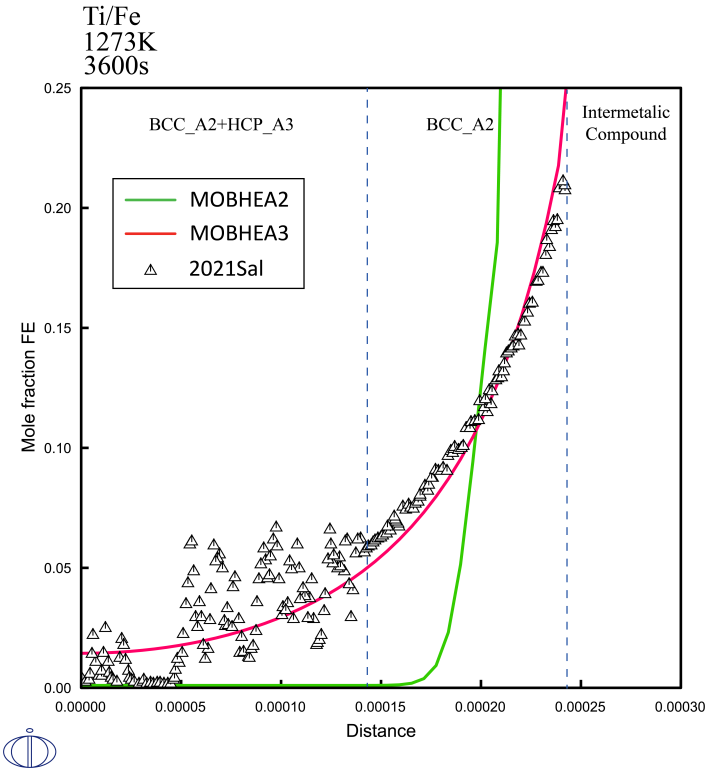

Figure 35: Simulated concentration profiles of Fe in the diffusion couple Fe/Ti annealed after 1 h at 1273 K compared with experimental data [2021Sal].

References

[2017Ver] V. Verma, A. Tripathi, K. N. Kulkarni, On Interdiffusion in FeNiCoCrMn High Entropy Alloy. J. Phase Equilibria Diffus. 38, 445–456 (2017).

[2019Che] W. Chen, L. Zhang, Experimental Investigations on the Quaternary Interdiffusion Coefficients, Young's Modulus and Hardness in bcc Ti-Nb-Ta-Zr Quaternary Alloys. J. Phase Equilibria Diffus. 40, 138–147 (2019).

[2021Sal] A. Salmasi, S. J. Graham, I. Galbraith, A. D. Graves, M. Jackson, S. Norgren, D. Guan, H. Larsson, L. Höglund, Mobilities of Ti and Fe in disordered TiFe-BCC assessed from new experimental data. Calphad. 74, 102300 (2021).

Precipitation Simulation (TC-PRISMA)

Combining the TCS High Entropy Alloys Database (TCHEA) with the compatible , TCS High Entropy Alloy Mobility Database (MOBHEA), the precipitation process can be simulated using the Precipitation Calculator, which is part of the Add-on Precipitation Module (TC-PRISMA) in Thermo-Calc. This example shows the Precipitation Calculator simulation of $L1_2$ precipitation in (NiCoFeCr)94Ti2Al4 FCC HEA matrix, in comparison with experimental information from [2018Zha].

Read more about the Precipitation Module (TC-PRISMA) on our website. If you are in Thermo-Calc, press F1 to search the help to learn about the available settings included with the Add-on Module.

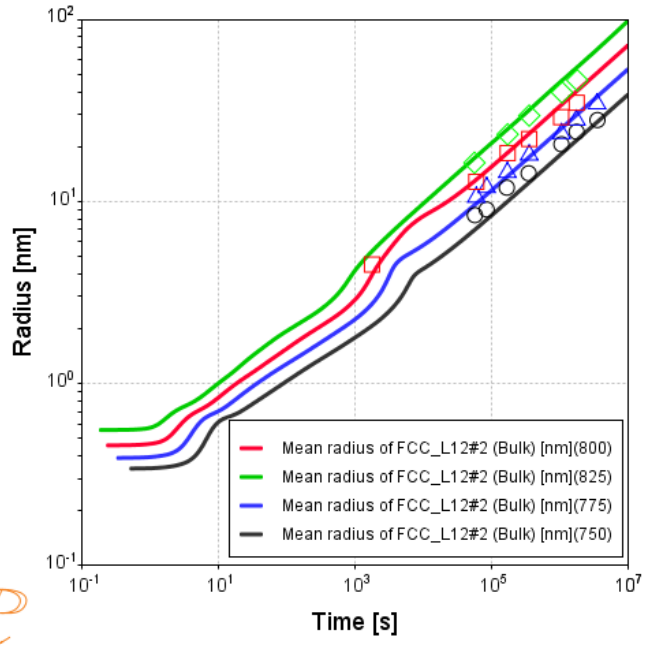

Figure 36: A Precipitation Module (TC-PRISMA) simulation of $L1_2$ precipitate from the (NiCoFeCr)94Ti2Al4 HEA matrix at various temperatures. This plot shows the mean radius of the $L1_2$ precipitates.

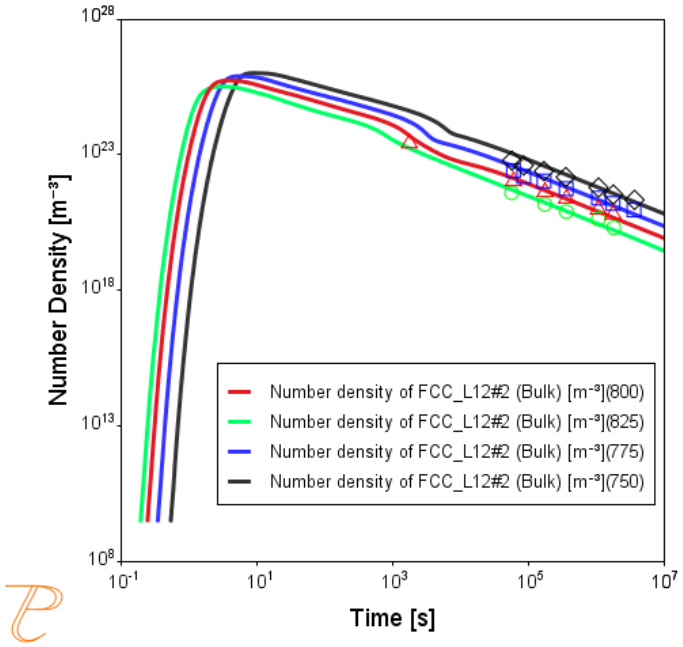

Figure 37: A Precipitation Module (TC-PRISMA) simulation of $L1_2$ precipitate from the (NiCoFeCr)94Ti2Al4 HEA matrix at various temperatures. This shows the number of densities of the $L1_2$ precipitates. Curves are using the Precipitation Calculator simulation results and symbols are experimental data from [2018Zha].

Reference

[2018Zha] Y. Y. Zhao, H. W. Chen, Z. P. Lu, T. G. Nieh, Thermal stability and coarsening of coherent particles in a precipitation-hardened (NiCoFeCr)94Ti2Al4 high-entropy alloy. Acta Mater. 147, 184–194 (2018).

TCHEA 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.

In this section:

Binary System Examples

The following plot examples using the TCS High Entropy Alloys Database (TCHEA) and for the Co-Cr, Co-Ni, Nb-Ti, and Fe-Ru binary systems show phase stabilities in the composition-temperature region. It can be used to guide the design of the compositions of BCC, FCC, and HCP medium- (MEA) or high- (HEA) entropy alloys and the relevant heat treatments.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our website or our YouTube playlist.

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

Co-Cr

The primary phase shifts from FCC in the Co-side to BCC in the Cr-side. The sigma phase is stable in the middle of this binary. The HCP phases are stable at low temperatures in Co-rich side.

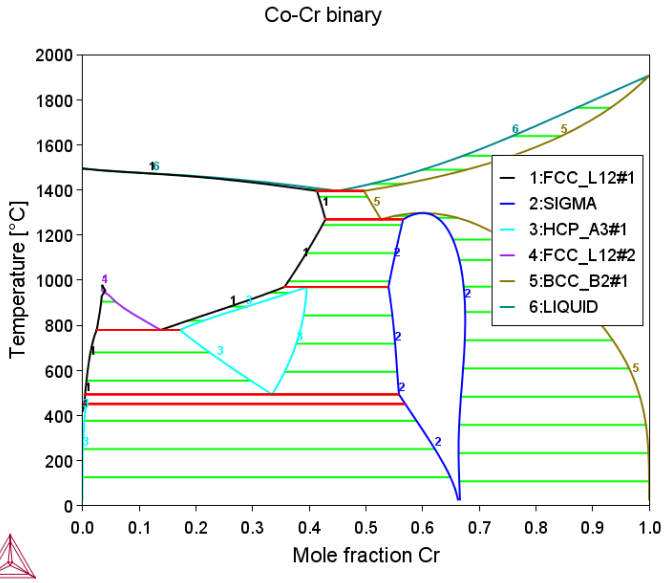

Figure 38: The Co-Cr binary phase diagram.

Co-Ni

The primary phase is FCC in the whole composition range. It is stable in a wide temperature range.

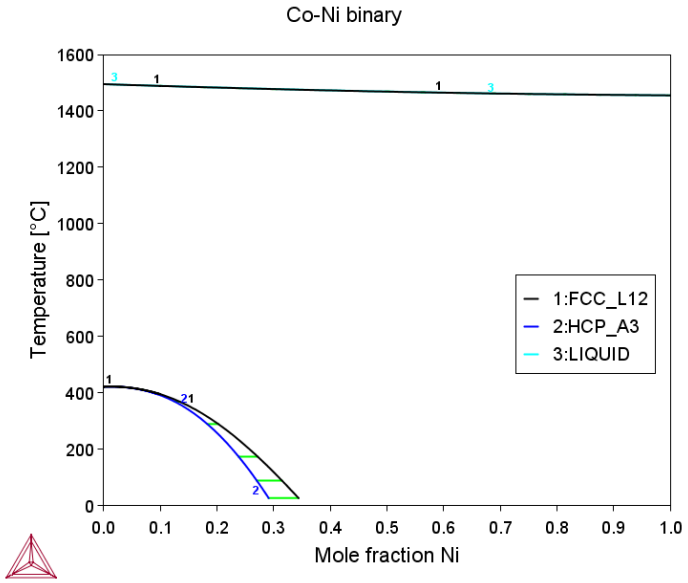

Figure 39: The Co-Ni binary phase diagram.

Nb-Ti

The primary phase is BCC in the whole composition range. It is stable in a wide temperature range.

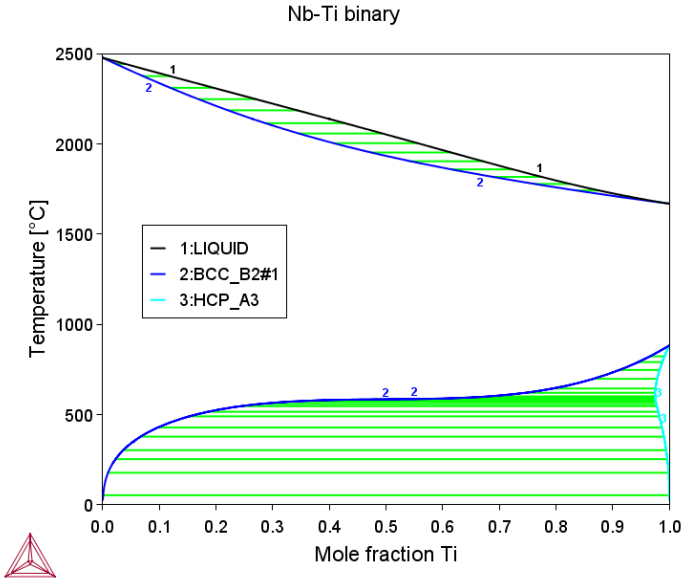

Figure 40: The Nb-Ti binary phase diagram.

Fe-Ru

The primary HCP phase has a wide composition and temperature range extending from the Ru-side.

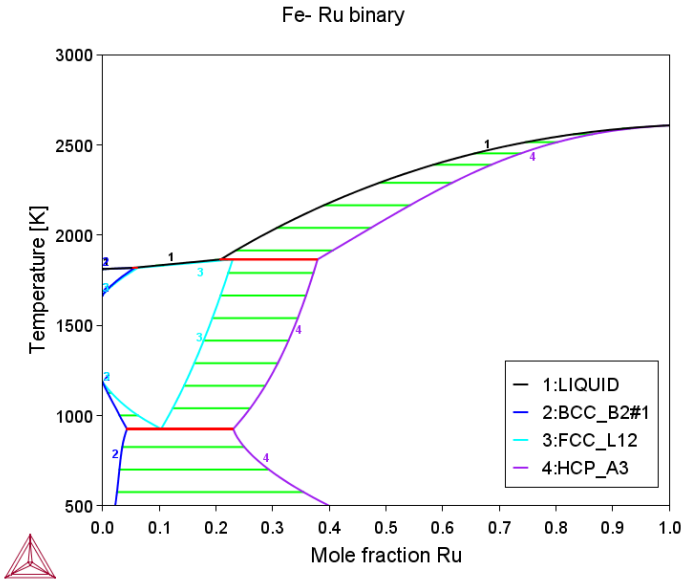

Figure 41: The Fe-Ru binary phase diagram.

Ternary System Examples

These ternary system examples using the TCS High Entropy Alloys Database (TCHEA) and for Co-Cr-Ni, Cr-Fe-Ni, and Nb-Ti-V show the phase stabilities in two dimensional plots, i.e. isothermal or vertical sections. It can be used to directly study medium entropy alloys (MEAs) or guide the design of high entropy alloys (HEAs).

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our website or our YouTube playlist.

Isothermal sections and liquidus projections for assessed ternary systems can be calculated using the Ternary Calculator in Graphical Mode or the TERNARY_DIAGRAM module in Console Mode. In Thermo-Calc press F1 to search the Help for more information.

Co-Cr-Ni

A vertical section, which is sometimes referred to as an *isopleth*, is a diagram showing the phase equilibria along a specific composition line and over a temperature range. These are often used to interpret the impact of the variation of composition on phase equilibria over temperatures or comparing the phase formation in a series of compositions during heating or cooling. Phase regions and boundaries among these are shown in a two-dimensional (2D) diagram.

Such a 2D diagram is similar to a binary phase diagram, but with an important difference: the level rule does not hold there. In other words, the phase boundaries of a two-phase region at specific temperatures in an ordinary isopleth do not correspond to the equilibrium compositions of the two phases. As shown in Figure 42, the alloy $Co_{0.25}Ni_{0.25}Cr_{0.50}$ is located in FCC_A1 + Sigma two-phase region at 1200 °C, which is adjacent to the FCC_A1 and Sigma single-phase regions. The boundaries just mark the end of the two-phase region, and the compositions are different from the equilibrium compositions of the two phases.

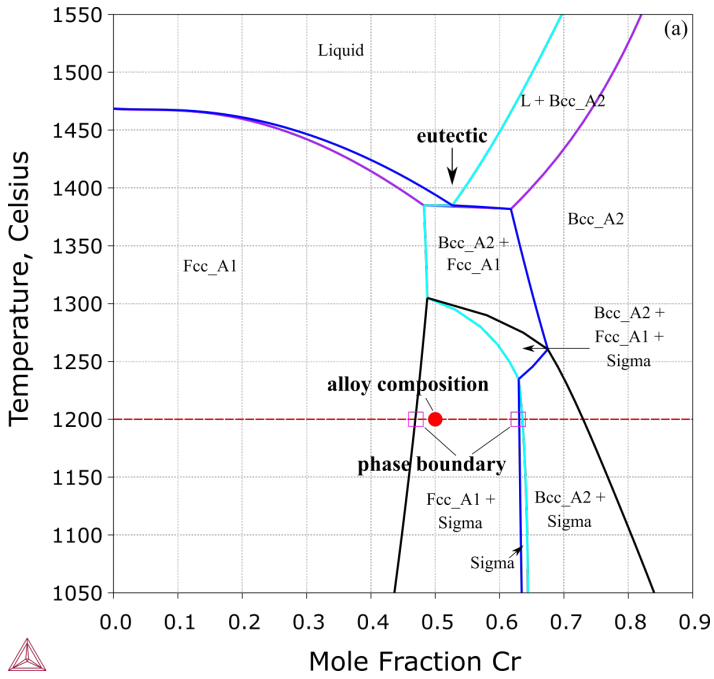

Figure 42: Equilibrium calculation of the extensively studied medium entropy alloy (MEA), the Co-Cr-Ni ternary system. This plot shows a vertical section from Cr0.5Ni0.5 to Cr [2018Che].

The tie-line, which stands for the composition line connecting the two equilibrium phases, is not confined within the vertical section. This can be clearly shown with an isothermal section at the same temperature as in Figure 43.

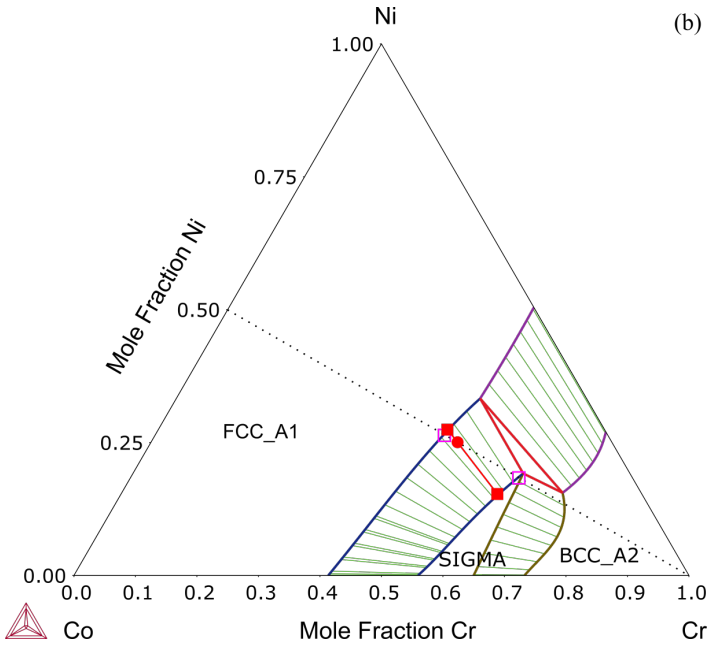

Figure 43: Equilibrium calculation of the extensively studied medium entropy alloy (MEA), the Co-Cr-Ni ternary system. This plot shows an isothermal section at 1200 °C. The alloy composition locates at Co0.25Ni0.25Cr0.50 [2018Che].

Cr-Fe-Ni

The Cr-Fe-Ni ternary provides a model system where the primary phase could either be BCC or FCC. The following equilibrium calculations—an isothermal section, the liquidus monovariant curve and the liquidus projection overlapping with a series of isothermal sections—can be used to design MEAs or HEAs with single phase (BCC or FCC) or dual-phase (BCC + FCC).

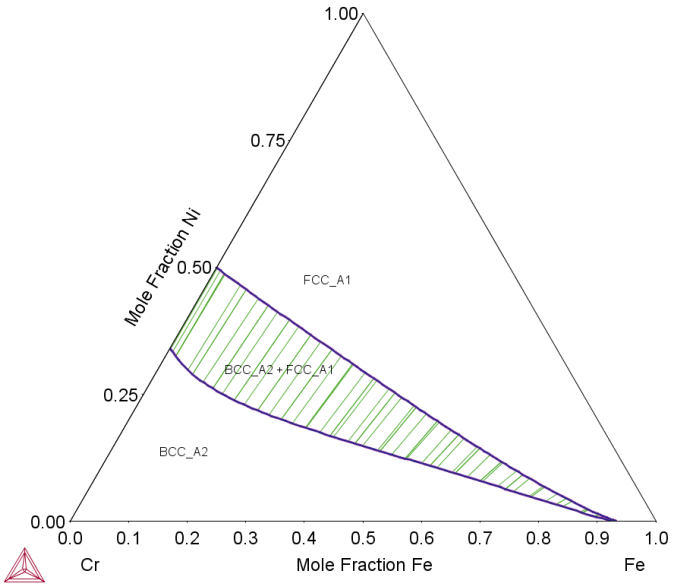

Figure 44: Equilibrium calculation of the Cr-Fe-Ni ternary with an isothermal section at 1300 °C.

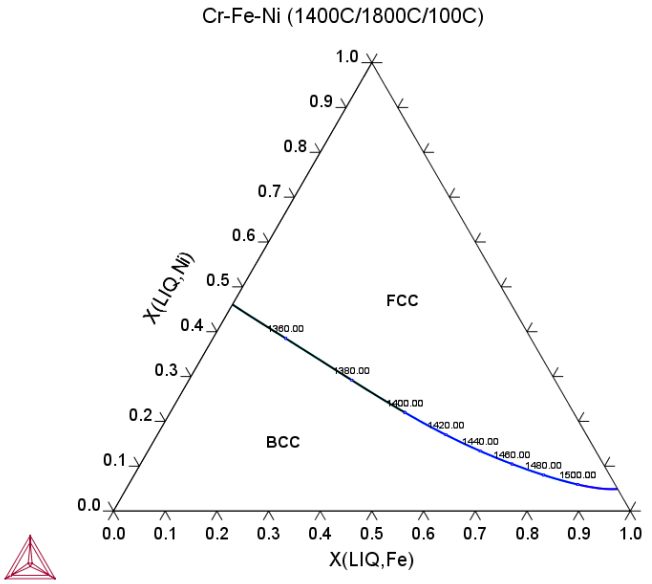

Figure 45: Equilibrium calculation of the Cr-Fe-Ni ternary showing a liquidus surface projection. The temperature (°C) value is plotted along the monovariant reaction curve. The primary phase shifts from BCC in Cr-corner to FCC in Ni-corner.

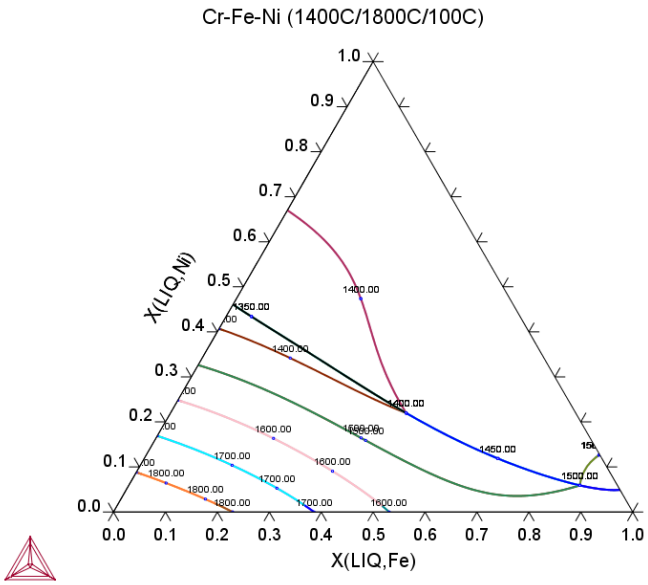

Figure 46: Equilibrium calculation of the Cr-Fe-Ni ternary with a liquidus projection overlapping with series of isothermal sections of the Cr-Fe-Ni ternary.

Nb-Ti-V

The Nb-Ti-V ternary system is important for the refractory BCC HEAs.

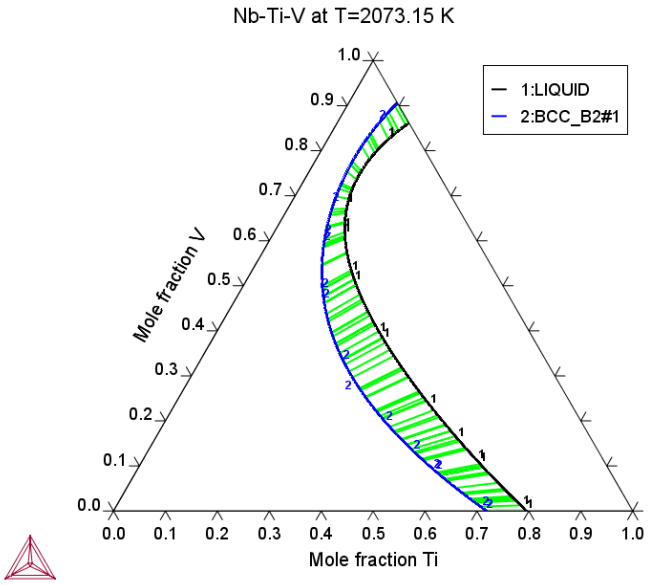

Figure 47: Isothermal section at 1800 °C of the Nb-Ti-V ternary.

Reference

[2018Che] H.-L. Chen, H. Mao, Q. Chen, Database development and Calphad calculations for high entropy alloys: Challenges, strategies, and tips. Mater. Chem. Phys. 210, 279–290 (2018).

Viscosity: Al-Cu, Al-Ni, and Cu-Ni-Al

Viscosity of liquid can be calculated directly using the TCS High Entropy Alloys Database (TCHEA) as a function of chemical composition and temperature.

The viscosity thermophysical property data is included with the TCS High Entropy Alloys Database (TCHEA) as of version 4 (TCHEA4).

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.

Al-Cu

The dynamic viscosity of Al-Cu binary system at 1373 K is calculated.

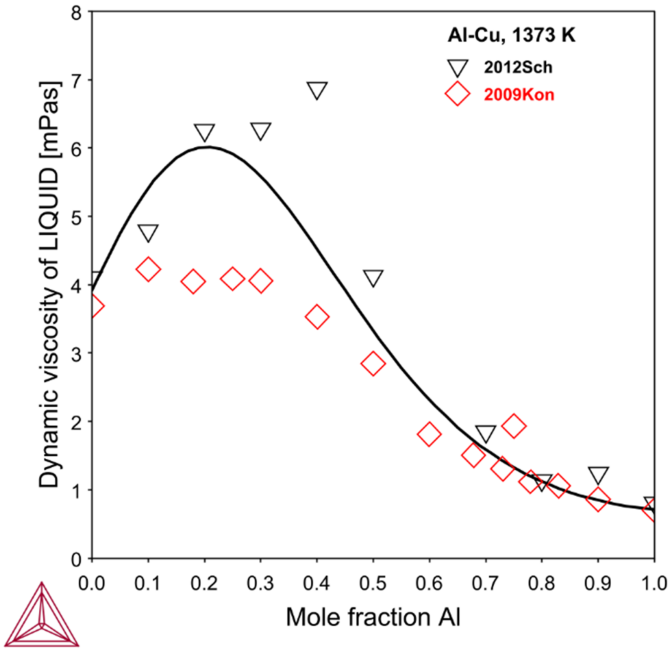

Figure 48: Calculated dynamic viscosity of Al-Cu at 1373 K along with experimental data from [2009Kon; 2012Sch].

Al-Ni

The dynamic viscosity of Al-Ni binary system at 1373 K is calculated in the following plot.

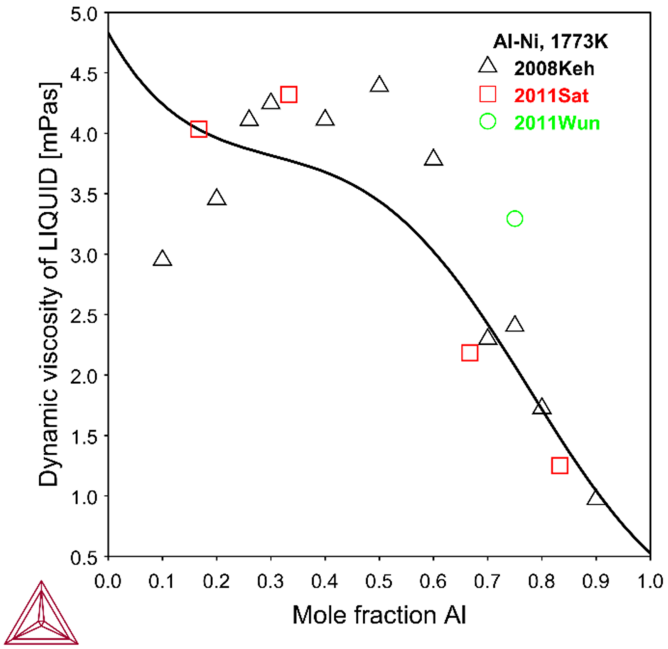

Figure 49: Calculated dynamic viscosity of Al-Ni at 1773 K along with experimental data from [2008Keh; 2011Sat; 2011Wun].

Cu-Ni-Al

The kinematic viscosity of equiatomic liquid alloys Cu-Ni-Al is shown.

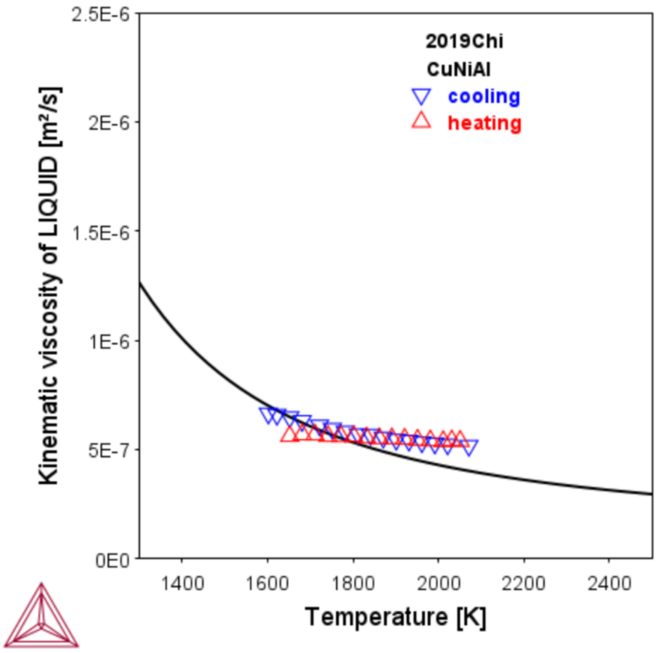

Figure 50: Calculated kinematic viscosity of equiatomic Cu-Ni-Al alloy along with experimental data from [2019Chi].

References

[2008Keh] M. Kehr, M. Schick, W. Hoyer, I. Ergy, Viscosity of the binary system Al-Ni. High Temp. - High Press. 37, 361–369 (2008).

[2009Kon] N. Y. Konstantinova, P. S. Popel', D. A. Yagodin, The kinematic viscosity of liquid copper-aluminum alloys. High Temp. 47, 336–341 (2009).

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[2011Wun] R. K. Wunderlich, H.-J. Fecht, Surface tension and viscosity of NiAl catalytic precursor alloys from microgravity experiments. Int. J. Mater. Res. 102, 1164–1173 (2011).

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[2019Chi] O. Chikova, V. Tsepelev, V. V'yukhin, K. Shmakova, V. Il'in, Viscosity and Electrical Resistivity of Liquid CuNiAl, CuNiAlCo, CuNiAlCoFe Alloys of Equiatomic Compositions. Acta Metall. Slovaca. 25, 259–266 (2019).