TCS Cu-based Alloys Database (TCCU)

Examples Collection

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 Cu-based Alloys Database (TCCU) 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 Cu-based Alloys Database (TCCU) Technical Information* PDF document contains version specific information such as the binary and ternary systems, phases and models. It also includes details about the 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 Cu-based Alloys Database (TCCU) 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 Copper-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 Copper 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.

TCCU 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 Phase Diagrams

Included binary systems in the TCS Cu-based Alloys Database (TCCU) are critically assessed based on available experimental and theoretical data for phase diagram and thermodynamic properties.

Some important key binary systems for copper-based alloys are shown here, for example, Cu-Zn, Cu-Sn, Cu-Be, and Cu-Ni systems.

> 📖 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 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.
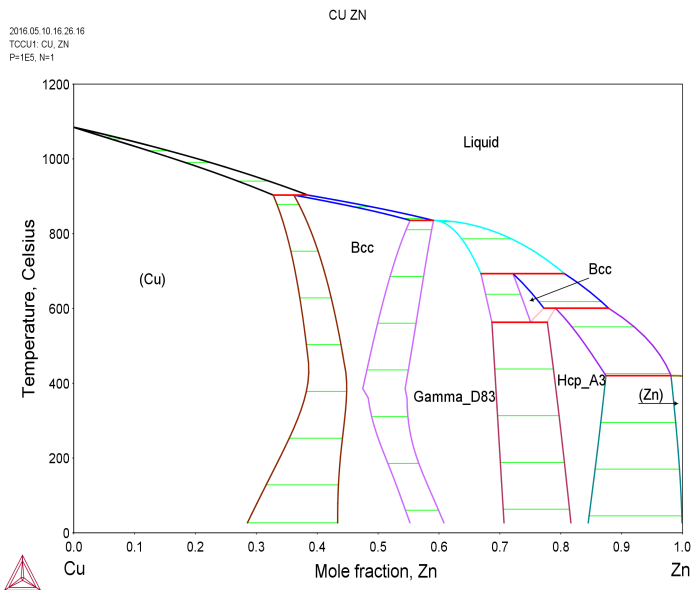

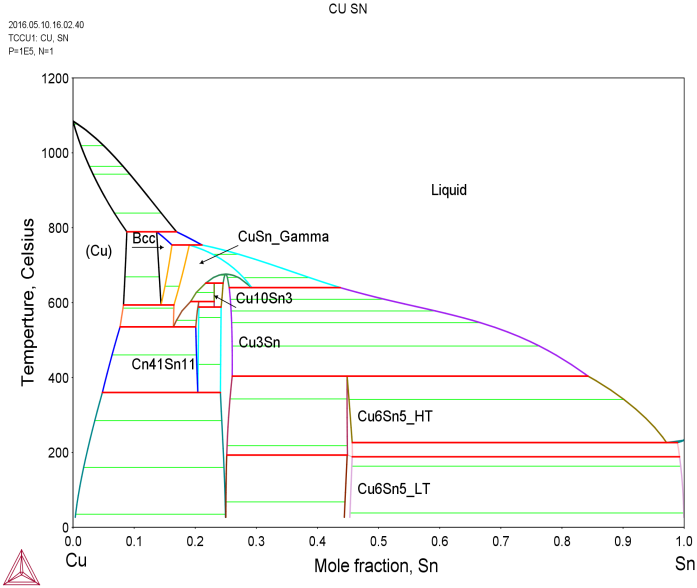*Figure 1: Calculated Cu-Zn phase diagram [2011Wan].*
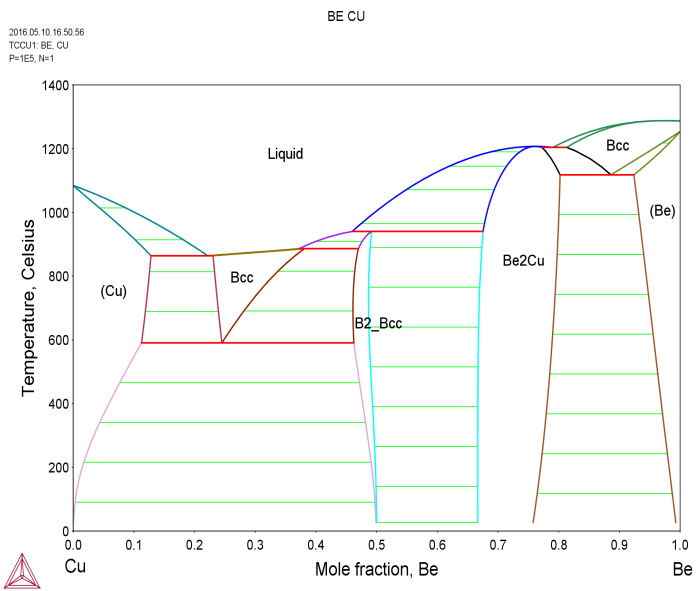
Figure 2: Calculated Cu-Sn phase diagram [2009Li].

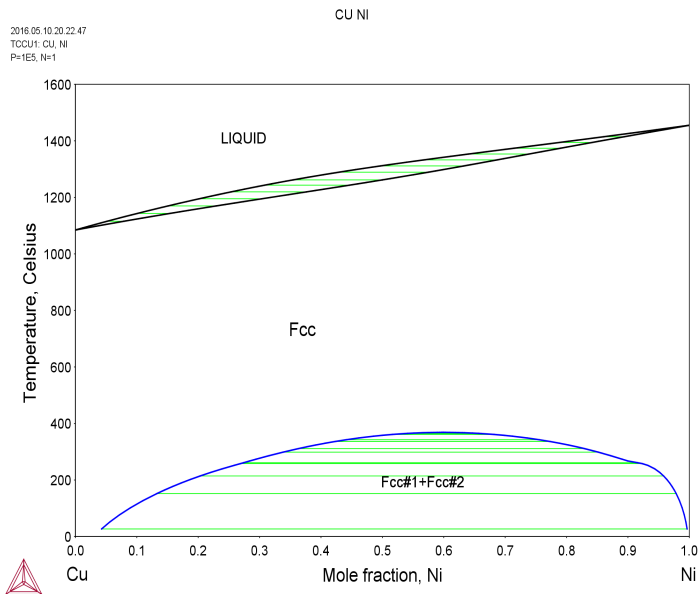*Figure 3: Calculated Cu-Be phase diagram.*

Figure 4: Calculated Cu-Ni phase diagram [1992anM].

References

[1992anM] S. an Mey, Thermodynamic re-evaluation of the Cu-Ni system. Calphad. 16, 255–260 (1992).

[2009Li] M. Li, Z. Du, C. Guo, C. Li, Thermodynamic optimization of the Cu–Sn and Cu–Nb–Sn systems. J. Alloys Compd. 477, 104–117 (2009).

[2011Wan] 1. J. Wang, H. Xu, S. Shang, L. Zhang, Y. Du, W. Zhang, S. Liu, P. Wang, Z.-K. Liu, Experimental investigation and thermodynamic modeling of the Cu–Si–Zn system with the refined description for the Cu–Zn system. Calphad. 35, 191–203 (2011).

Isothermal Sections

Typical ternary phase diagrams are isothermal and vertical sections. Such diagrams can be of practical applications as well, e.g. making a preliminary determination of the heating temperature for melting, solution treatment, homogenization, and aging for specific alloys.

In these examples, the isothermal sections for Cu-Mn-Sn system at 550 °C and Cu-Ni-Sn system at 800 °C are calculated with the TCS Cu-based Alloys Database (TCCU). The experimental data are appended for comparison.

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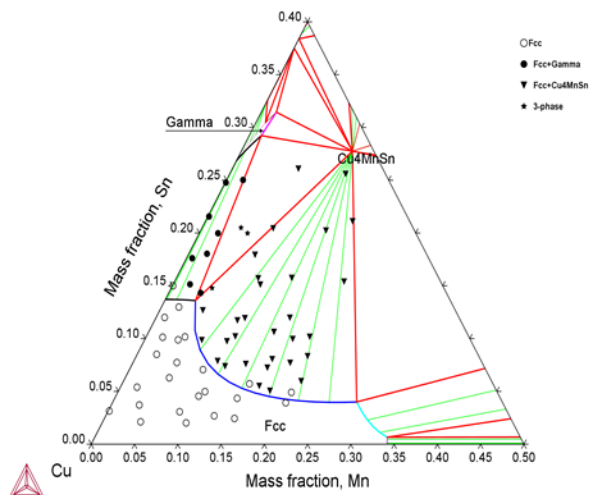

Figure 5: Calculated isothermal section of Cu-Mn-Sn at 550°C along with experimental data [1953Bla; 1953Fun; 1987Leo].
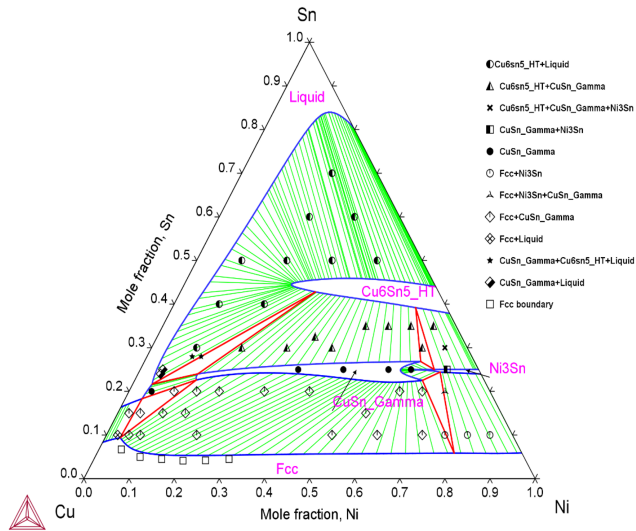
Figure 6: Calculated isothermal section of Cu-Ni-Sn at 800 °C along with experimental data [2003Wan].

References

[1953Fun] C. W. Funk, J. A. Rowland, Alpha Solid-Solution Area of the Cu-Mn-Sn System. Trans. Am. Soc. Met. AIME. 197, 723–725 (1953).

[1953Bla] J. C. Blade, J. W. Cuthbertson, The structure and mechanical properties of copper-manganese. J. Inst. Met. 82, 17–24 (1953).

[1987Leo] N. P. Leonova, N. R. Bochvar, E. V Lysova, Phase equilibria in copper-rich Cu-Mn-Sn alloys. Russ. Metall. 4, 204–206 (1987).

[2003Wan] C.-H. Wang, S.-W. Chen, Isothermal section of the ternary Sn-Cu-Ni system and interfacial reactions in the Sn-Cu/Ni couples at 800 °C. Metall. Mater. Trans. A. 34, 2281–2287 (2003).

Vertical Sections

Typical ternary phase diagrams are isothermal and vertical sections. Such diagrams can be of practical applications as well, e.g. making a preliminary determination of the heating temperature for melting, solution treatment, homogenization, and aging for specific alloys.

The vertical sections of Cu-Mn-Zn ternary system with 10 wt.% Mn, Cu-Co-Fe ternary system with Fe:Co = 1:3, and Cu-Ce-Ni ternary system with 9 at.% Ce are each calculated using the TCS Cu-based Alloys Database (TCCU). Comparisons between the experimental data and the calculations are included.

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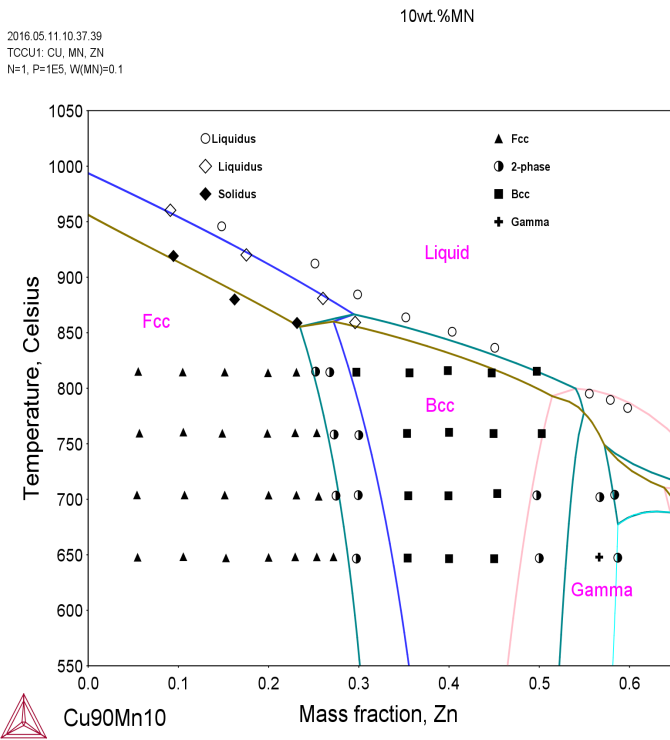

Figure 7: Calculated vertical section 10wt.% Mn in the Cu-Mn-Zn system along with the experimental data [1927Heu; 1949Gra; 1972Wat].
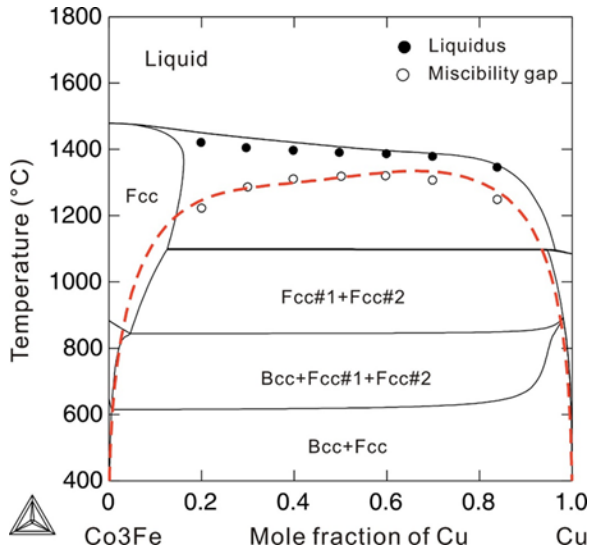
Figure 8: Calculated vertical section Fe:Co = 1:3 (at.%) in the Cu-Co-Fe system along with the experimental data [2005Cao]. The red dashed line is the metastable liquid miscibility gap.
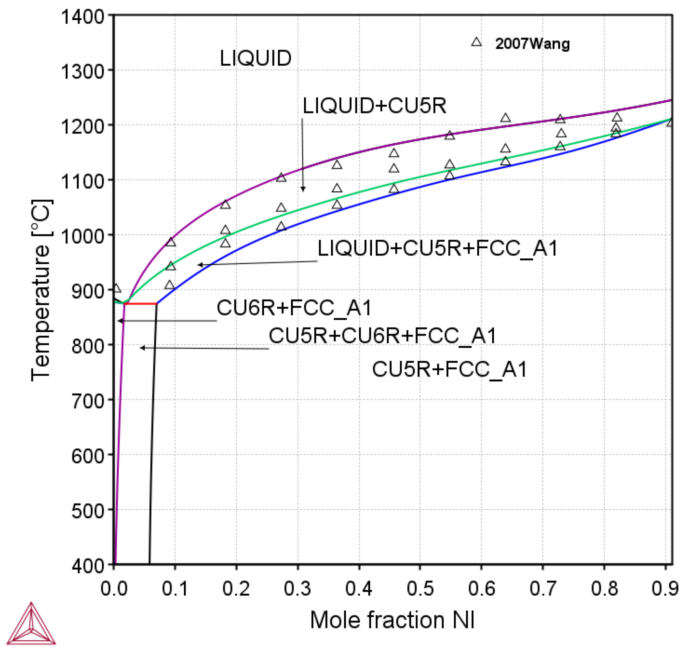

Figure 9: The calculated vertical section with 9 at.% Ce in Cu-Ce-Ni system along with the experimental data [2007Wan].

References

[1927Heu] O. Heusler, Über das ternäre System Kupfer-Zink-Mangan. Zeitschrift fur Anorg. und Allg. Chemie. 159, 37–54 (1927).

[1949Gra] T. R. Graham, J. R. Long, C. E. Armantrout, A. H. Roberson, The ternary system, copper-manganese-zinc. Trans. Am. Inst. Min. Met. Pet. Eng. 185, 675–682 (1949).

[1972Wat] H. Watanabe, N. Kono, M. Gonda, A Study of the Phase Diagram of the Ternary Cu-Zn-Mn System (in Japanese). J. Japan Inst. Met. 36, 297–305 (1972).

[2005Cao] C.-D. Cao, G. P. Görler, Direct Measurement of the Metastable Liquid Miscibility Gap in Fe–Co–Cu Ternary Alloy System. Chinese Phys. Lett. 22, 482–484 (2005).

[2007Wan] J. Wang, A. Pisch, R. Flükiger, J. L. Jorda, Phase equilibrium in the cerium-poor Ce–Ni–Cu system. J. Alloys Compd. 436, 161–169 (2007).

Liquidus Projection

The liquidus projection of Cu-Ag-Sn ternary system are shown using the TCS Cu-based Alloys Database (TCCU). Comparison between the experimental data and the calculations are included.

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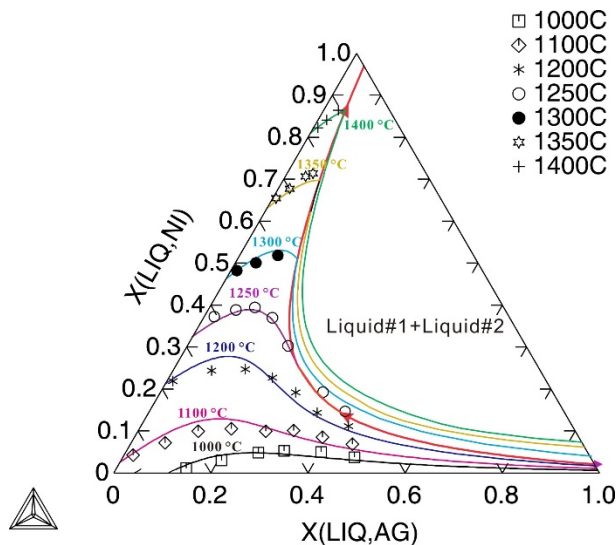

Figure 10: Calculated liquidus projection along with experimental data [199Kub] in the Cu-Ag-Ni system [2008Liu].

References

[1998Kub] O. Kubaschewski, Silver-Copper-Nickel in Ternary Alloy Phase Diagrams, G. Petzow, G. Effenberg, Eds., pp. 596–604, (1998).

[2008Liu] X. J. Liu, F. Gao, C. P. Wang, K. Ishida, Thermodynamic Assessments of the Ag-Ni Binary and Ag-Cu-Ni Ternary Systems. J. Electron. Mater. 37, 210–217 (2008).

Thermodynamic Properties

The TCS Cu-based Alloys Database (TCCU) can satisfactorily predict thermodynamic properties of various copper alloys. In this example, the mixing enthalpies of various Cu-Ni-Sn melts at 1583 K are calculated and compared with experimental data [1979Poo].
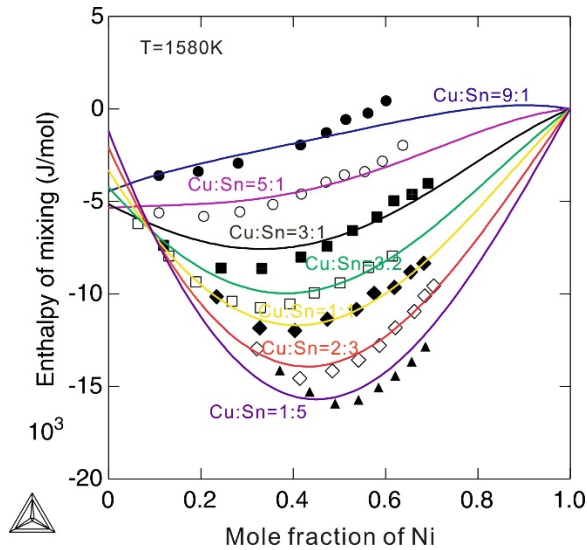

Figure 11: Mixing enthalpies of liquid phase in the Cu-Ni-Sn system at 1583 K compared with experimental data [1979Poo].

Reference

[1979Poo] M. J. Pool, I. Arpshofen, B. Predel, E. Schultheiss, Ermittlung von Mischungsenthalpien fluessiger Legierungen des Systems Cu-Ni-Sn mit einem SETARAM-Hochtemperatur-Kalorimeter. Zeitschrift für Met. 70, 656–659 (1979).

Density and Molar Volume

The TCS Cu-based Alloys Database (TCCU) contains a database of molar volume and thermal expansion coefficients of all phases. By applying the TCCU database, the molar volume and the density can be well predicated. In this example, the density of various Cu-Co-Fe melts varying with temperatures was calculated with TCCU and Thermo-Calc.
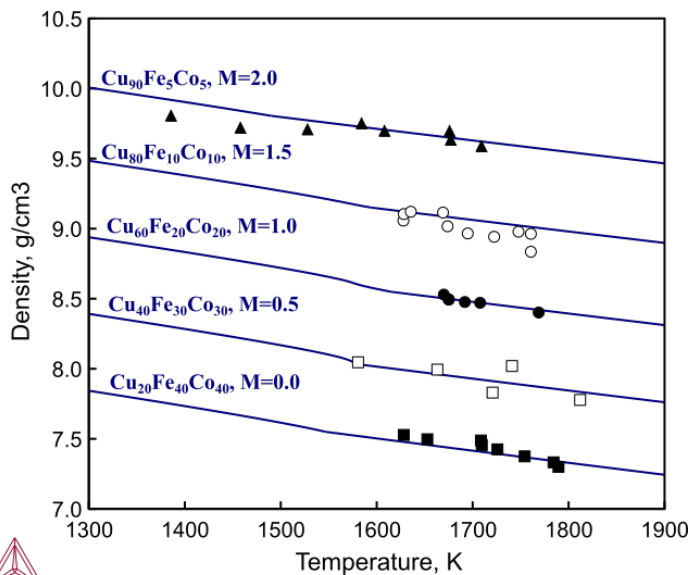

Figure 12: Calculated density of liquid Cu-Co-Fe alloys. Symbols are the experimental values from [2006Bri]. A constant, M, is added in order to separate the data.

Reference

[2006Bri] J. Brillo, I. Egry, T. Matsushita, Density and excess volumes of liquid copper, cobalt, iron and their binary and ternary alloys. Int. J. Mater. Res. 97, 1526–1532 (2006).

Surface Tension: Ag-Cu and Ag-Au-Cu

The surface tension thermophysical property data is included with the TCS Cu-based Alloys Database (TCCU) as of version 4 (TCCU4).

For more information about the various thermophysical 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](#).
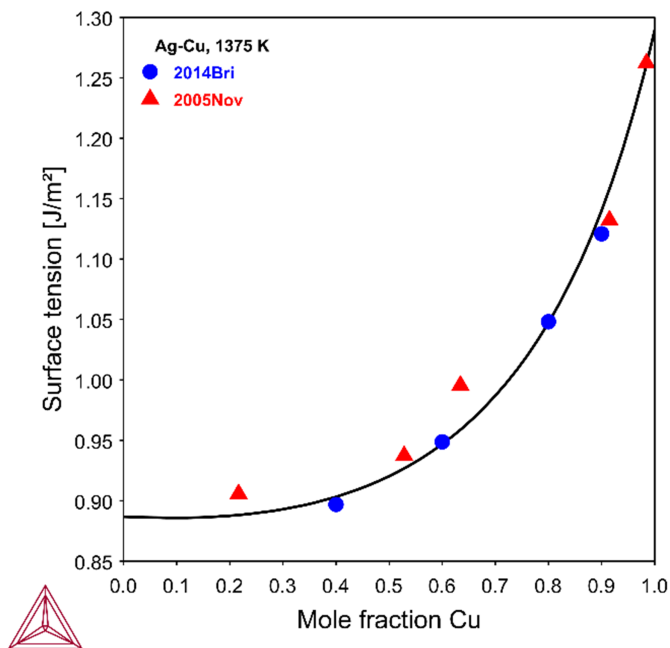
Ag-Cu

Figure 13: Surface tension of Ag-Cu at 1375 K. Experimental data are taken from [2005Nov; 2014Bri].

Ag-Au-Cu

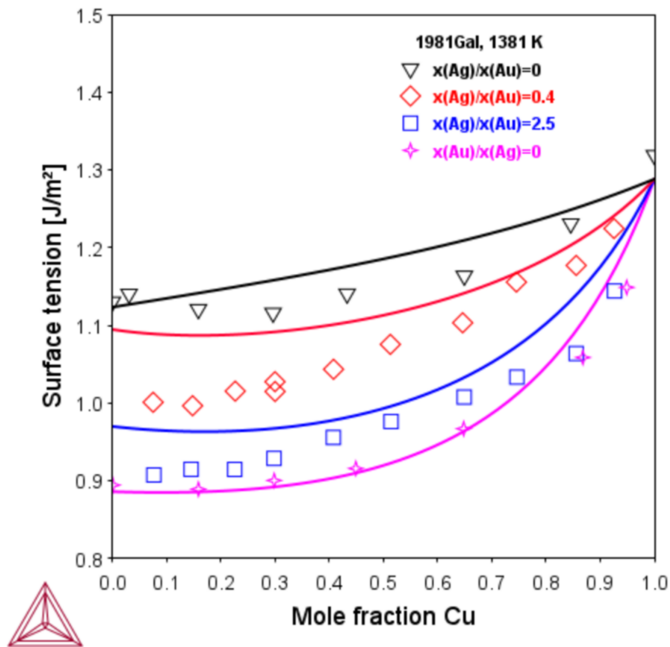The surface tensions of several liquid Ag-Au-Cu alloys are shown.

Figure 14: Calculated surface tension of Ag-Cu, Au-Cu and Ag-Au-Cu alloys at 1381 K along with experimental data from [1981Gal].

References

[1981Gal] B. Gallois, C. H. P. Lupis, Surface tensions of liquid Ag-Au-Cu alloys. Metall. Trans. B. 12, 679–689 (1981).

[2005Nov] R. Novakovic, E. Ricci, D. Giuranno, A. Passerone, Surface and transport properties of Ag–Cu liquid alloys. Surf. Sci. 576, 175–187 (2005).

[2014Bri] J. Brillo, G. Lauletta, L. Vaianella, E. Arato, D. Giuranno, R. Novakovic, E. Ricci, Surface Tension of Liquid Ag–Cu Binary Alloys. ISIJ Int. 54, 2115–2119 (2014).

Viscosity: Al-Cu, Cu-Fe, and Al-Cu-Fe

The viscosity thermophysical property data is included with the TCS Cu-based Alloys Database (TCCU) as of version 4 (TCCU4).

For more information about the various thermophysical 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 and Cu-Fe

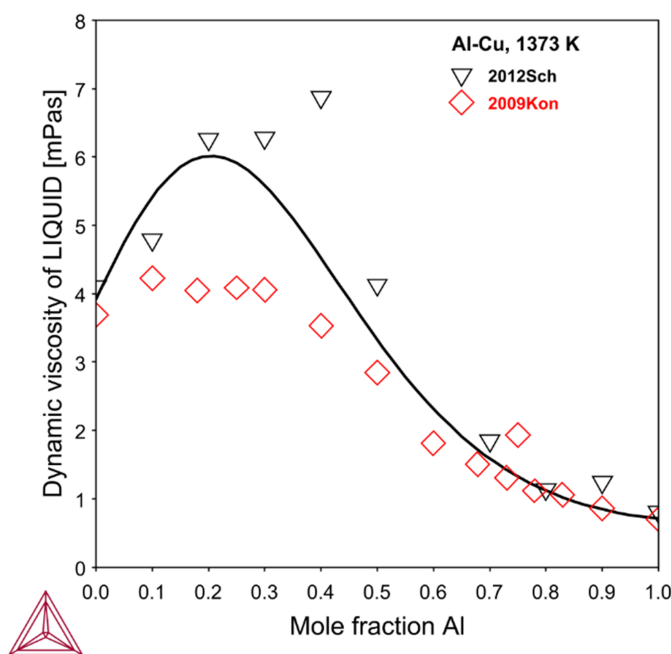The dynamic viscosity of Al-Cu binary system at 1373 K is calculated in the following plot.

Figure 15: Calculated dynamic viscosity of Al-Cu at 1373 K along with experimental data from [2009Kon; 2012Sch].

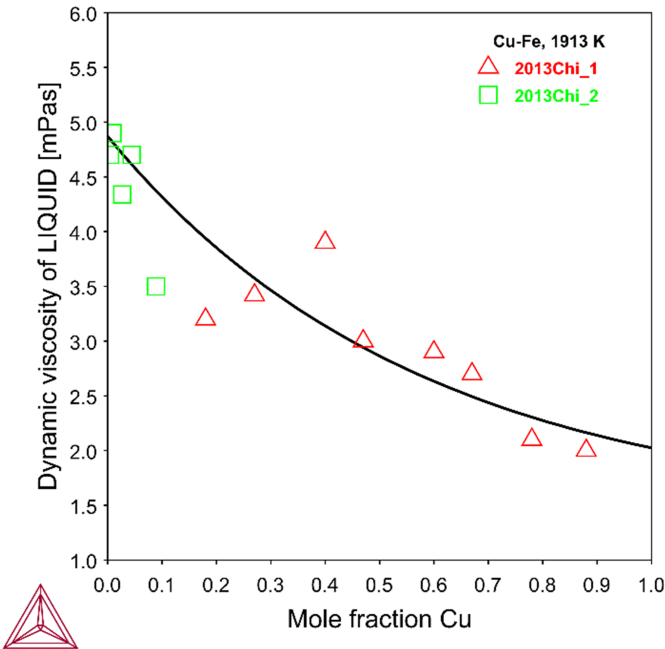The dynamic viscosity of Cu-Fe binary system at 1913 K is calculated in the following plot.

Figure 16: Calculated dynamic viscosity of Cu-Fe at 1913 K along with experimental data from [2013a/bChi].

Al-Cu-Fe

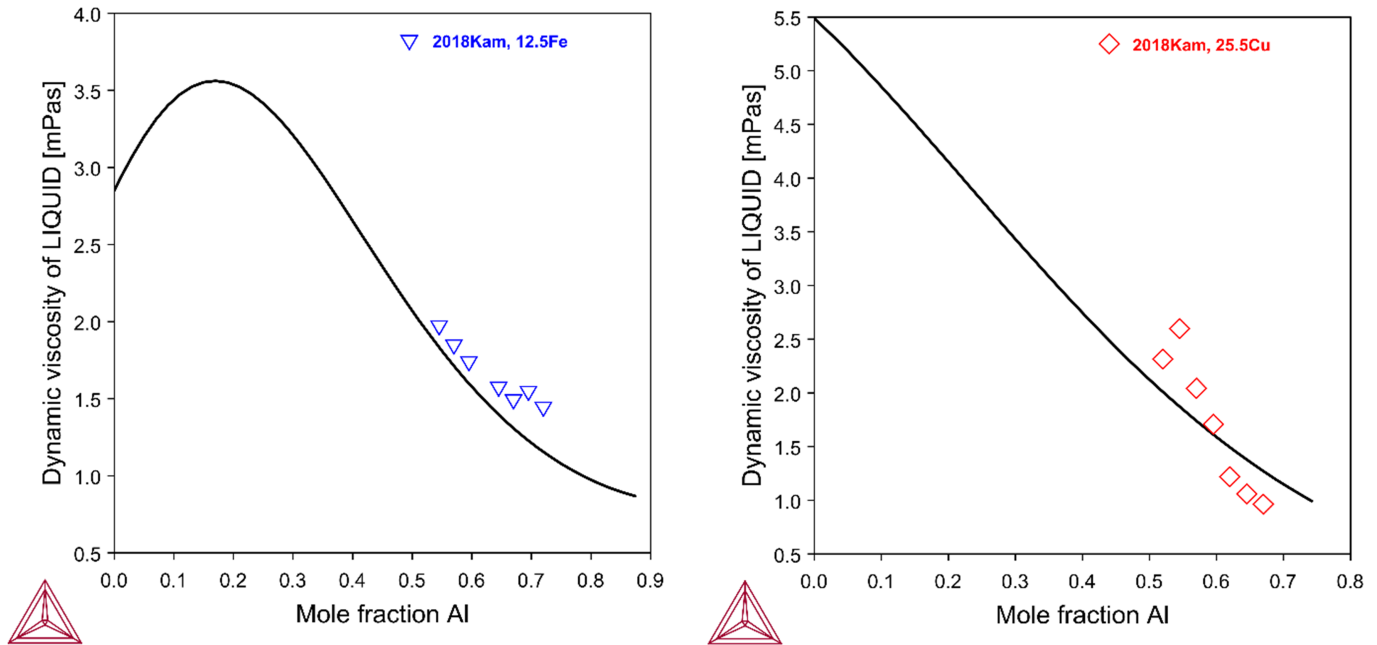The following shows the kinematic viscosity as a function of Al composition.

Figure 17: Kinematic viscosity of Al-Cu-Fe alloys at 12.5 at% Fe (left) and 25.5 at% Cu (right) along with experimental data from [2018Kam].

References

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

[2012Sch] M. Schick, J. Brillo, I. Egry, B. Hallstedt, Viscosity of Al–Cu liquid alloys: measurement and thermodynamic description. J. Mater. Sci. 47, 8145–8152 (2012).

[2013aChi] O. A. Chikova, V. S. Tsepelev, A. N. Konstantinov, V. V V'yukhin, Influence of copper additives on the viscosity and stratification of iron melt. Steel Transl. 43, 262–266 (2013).

[2013bChi] O. A. Chikova, V. S. Tsepelev, A. N. Konstantinov, V. V V'yukhin, Viscosity and separation of Fe-Cu melts. Russ. Metall. 2013, 643–646 (2013).

[2018Kam] L. V. Kamaeva, A. Y. Korepanov, V. I. Lady'anov, Temperature Behavior of the Viscosity of Quasi Crystal-Forming Al–Cu–Fe Melts. High Temp. 56, 514–518 (2018).

TCCU 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:

Liquidus and Solidus Temperatures

The TCS Cu-based Alloys Database (TCCU) can be used to predict the liquidus and solidus temperatures, as well as incipient melting temperatures, which are critical to design heat treatments and melting processes.

The liquidus and solidus temperatures for more than 110 commercial copper-based alloys have been collected and compared to the calculated temperatures using TCCU.

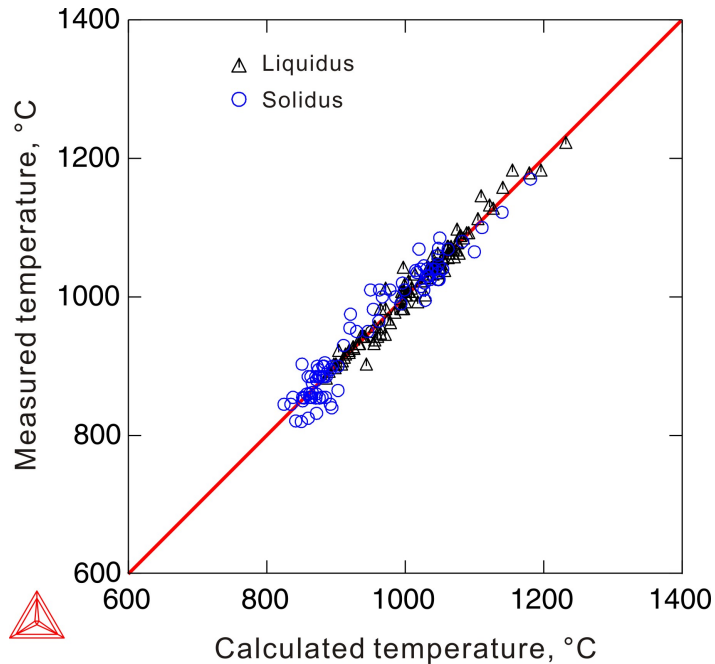*Figure 18: Comparison of calculated and experimental [2001Dav] liquidus and solidus temperatures for various industry copper alloys.*

Reference

[2001Dav] J. R. Davis, Copper and Copper Alloys: ASM Specialty Handbook (ASM International, 2001).

Solidification Simulations

Solidification is one of the most critical processes in copper alloys; it determines the formation of the bulk microstructure and then directly affects the mechanical and chemical properties of the alloys. Thus, being able to accurately simulate the solidification behavior of a copper alloy is of great importance.

With solidification simulations, the phase formation sequence, phase fraction, phase transformation temperatures, and so forth, can be predicted using Thermo-Calc and the TCS Cu-based Alloys Database (TCCU).

Scheil Solidification Simulations

A conventional Scheil simulation provides an upper boundary for how far a solidification can deviate from equilibrium, therefore a real solidification is expected to occur between the equilibrium simulation and the Scheil simulation.

The plot simulates both the equilibrium solidification and Scheil (non-equilibrium) solidification of a Cu-5.2 wt.%Sn-4.7wt.%Pb alloy. The calculated Scheil solidification path, including the solidified phases and the phase transformation temperatures, agrees well with the experimental data [2009Kor].

> Read more about Scheil Solidification Simulations on our website. If you are in Thermo-Calc, press F1 to search the help to learn about using Scheil.
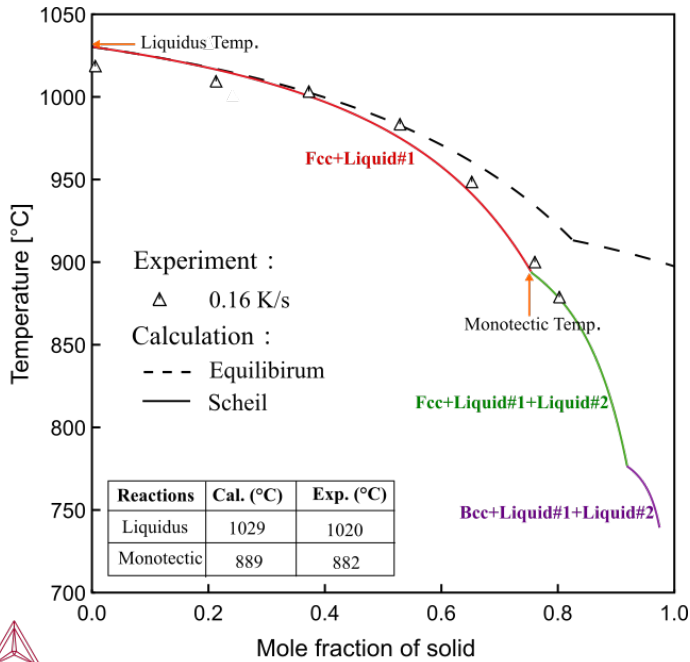
Figure 19: Equilibrium solidification and Scheil solidification simulations of Cu-5.2 wt.%Sn-4.7wt.%Pb alloy, compared with experimental result [2009Kor]. The calculated Scheil solidification path, including the solidified phases and the phase transformation temperatures, agrees well with the experimental data.

Microsegregation Simulation

Microsegregation occurs from solute partitioning during solidification processes. In addtion to causing an inhomogenous microstructure, microsegregation can cause the formation of phases that were not predicted on the equilibrium phase diagram, which could lead to defects or undesirable mechanical properties.

Using both the TCS Cu-based Alloys Database (TCCU) and TCS Cu-based Alloys Mobility Database (MOBCU), the microsegregation process in copper alloys can be modeled using the Add-on Diffusion Module (DICTRA).

> Read more about the Diffusion Module (DICTRA) 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.

In this example, the microsegregation behaviors of Cu-4.9wt.%Pb-5.2wt.%Sn-4.5wt.%Zn during the solidification was predicted in a Diffusion Module (DICTRA) solidification simulation. The concentration of solute Sn and Zn increases from the central to the edge of the dendrite in Cu-4.9wt.%Pb-5.2wt.%Sn-4.5wt.%Zn alloys, while that of Cu shows a decreased trend.
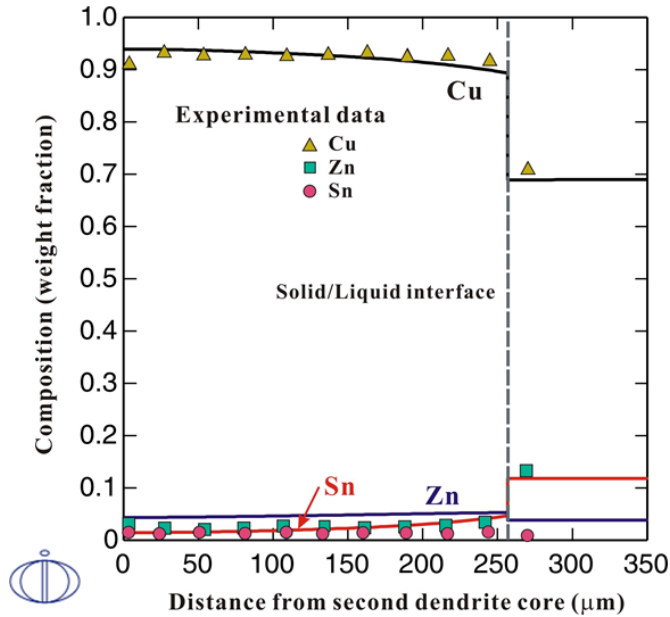
Figure 20: Calculated composition profile through half dendrite cross section in Cu-4.9wt.%Pb-5.2wt.%Sn-4.5wt.%Zn alloy during the solidification process along with experimental data [2009Kor]. The cooling rate is 0.16 °C/s.

References

[2009Kor] B. Korojy, L. Ekbom, H. Fredriksson, Microsegregation and Solidification Shrinkage of Copper-Lead Base Alloys. Adv. Mater. Sci. Eng. 2009, 1–9 (2009).

[2018Tan] Y. Tang, Q. Chen, A. Engström, Kinetic simulations of diffusion-controlled phase transformations in Cu-Based alloys, In L.J. Zhang (Ed.), Modeling of diffusion-controlled phase transformation in alloys, Diffusion Foundation, Tans Tech Publications Ltd, 2018, pp. 1-22.

Precipitation Simulations

Precipitation particle size and its distribution have a decisive influence on the subsequent mechanical properties of high-strength and highly conductive precipitation hardened copper alloys. With a combination of TCS Cu-based Alloys Database (TCCU) and TCS Cu-based Alloys Mobility Database (MOBCU), the average size and number density, as well as volume fraction of a precipitate, can be predicted by using the Precipitation Module (TC-PRISMA) in Thermo-Calc.

> 📖 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.

Precipitation in Cu-Ni-Si Alloy

The Cu-Ni-Si alloy is a precipitation strengthening-type alloy and receives a lot of attention for its high strength and high electrical conductivity. In this example, the precipitation simulation is carried out in Cu-1.86 wt.% Ni-0.45 wt.% Si alloy at 948 K, from which a rod-shape precipitate (Ni_2Si) precipitates in (Cu) matrix.

The simulated mean length (red line) and mean width (black line) of Ni_2Si precipitates agree well with the measured values [2011Wat].
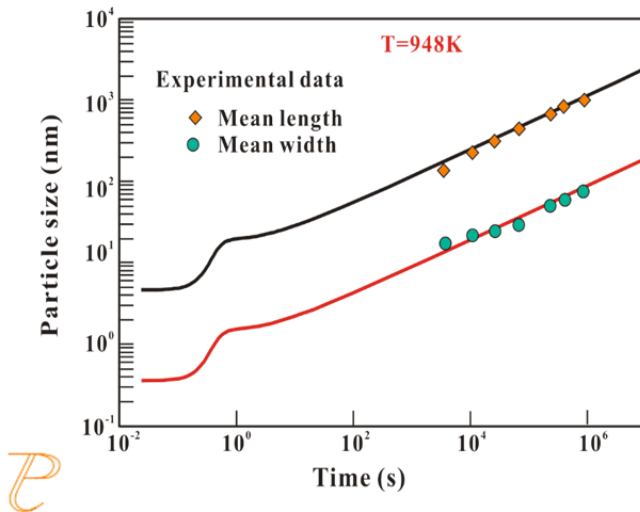

Figure 21: Simulated average length (red line) and width (black line) of rod-shaped precipitates with aging time for Cu-1.86wt.%Ni-0.45wt.%Si alloy at 948K compared with reported experimental data [2011Wat].

Precipitation in Cu-Co-Fe Alloy

In this example, the precipitation simulation is carried out in Cu-0.68 at.%Co-1.52 at.%Fe alloy during the isothermal aging process at 973, 923, and 873 K. During the aging treatment, the fcc Co-Fe precipitates in (Cu) matrix. Based on the experimental observation, the shape of the particles could change from sphere to cuboid when the particles become large. Due to the absence of the cubic factor, the morphological evolution is ignored in the simulation. The normalized particle size distributions (PSD) for the 973 K precipitation at 0.5 h are simulated and compared with the measurements [2009Wat]. The number density at various temperatures are also obtained for the fcc Co-Fe precipitate in Cu-0.68 at.%Co-1.52 at.%Fe alloy. Good agreement between the predictions and measurements can be observed.
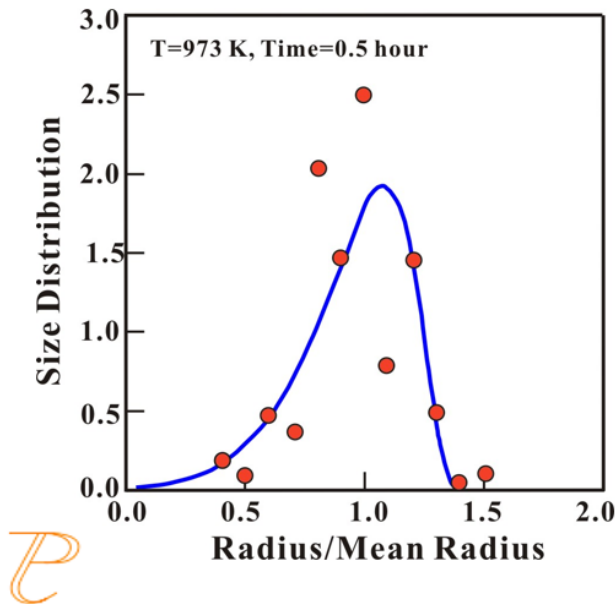

Figure 22: Comparison of the simulated particle size distribution of fcc Co-Fe precipitates in Cu-0.68 at.%Co-1.52 at.%Fe alloy annealed at 973 K for 0.5 h with the experimental data [2011Wat].
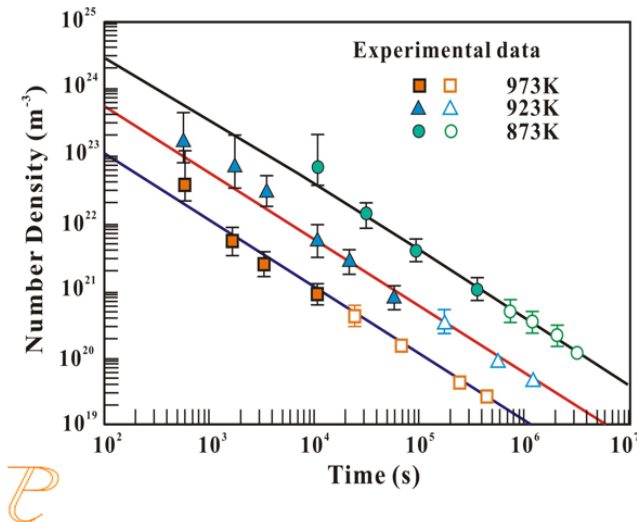
Figure 23: Simulated and experimental number density of fcc Co-Fe precipitate in Cu- 0.68 at.%Co-1.52 at.%Fe alloy annealed at 973, 923, and 873 K. The solid symbols are experimental data [2009Wat] for spherical particles; and the open symbols are for cuboid particles.

References

[2009Wat] D. Watanabe, C. Watanabe, R. Monzen, Determination of the interface energies of spherical, cuboidal and octahedral face-centered cubic precipitates in Cu-Co, Cu-Co-Fe and Cu-Fe alloys, Acta Metal. 57, 1899–1911 (2009).

[2011Wat] C. Watanabe, R. Monzen, Coarsening of δ-Ni2Si precipitates in a Cu-Ni-Si alloy, J. Mater. Sci. 46, 4327–4335 (2011).

[2018Tan] Y. Tang, Q. Chen, A. Engström, Kinetic simulations of diffusion-controlled phase transformations in Cu-Based alloys, In L.J. Zhang (Ed.), Modeling of diffusion-controlled phase transformation in alloys, Diffusion Foundation, Tans Tech Publications Ltd, 2018, pp. 1-22.

[2020Che] Q. Chen, Y. Tang, A. Engström, Developing Thermodynamic and Kinetic Databases for Cu–Based Alloy Design. J. Japan Inst. Copp. 59, 7–12 (2020).

Viscosity of L68 Brass Melts

The viscosity thermophysical property data is included with the TCS Cu-based Alloys Database (TCCU) as of version 4 (TCCU4).

For more information about the various thermophysical 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 viscosity is a critical material property needed when performing finite element simulations of casts or welds. Thermophysical data found in handbooks and finite element (FE) codes typically does not capture chemistry variation or data for novel/experimental materials. Below is the calculated viscosity for a specific chemistry of L68 brass compared with some measured values.
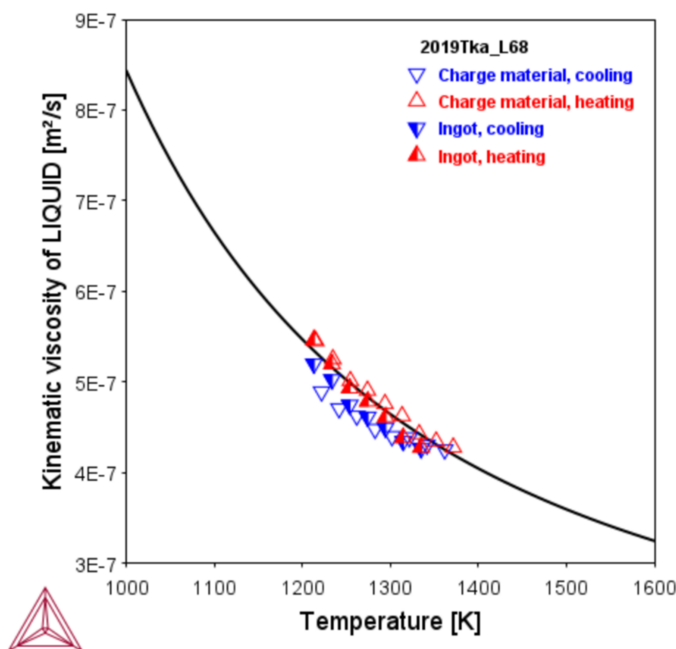

Figure 24: Calculated kinematic viscosities of the melts of L68 brass along with experimental data from [2019Tka].

Reference

[2019Tka] G. A. Tkachuk, O. A. Chikova, V. V. V'yukhin, Viscosity of Molten Brass and Copper Used for Quality Control in the Charge–Melt–Ingot Chain. Russ. Metall. 2019, 1220–1223 (2019).