Thermo-Calc Software

TCS Noble Metal Alloys Database (TCNOBL)

Examples Collection

Document created 6/21/2023

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 Noble Metal Alloys Database (TCNOBL) 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 Noble Metal Alloys Database (TCNOBL) 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 Noble Metal Alloys Database (TCNOBL) 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 Noble Metal 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 Precious Metals 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.

TCNOBL 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:

Isothermal and Vertical Sections

Included ternary systems in the TCS Noble Metal Alloys Database (TCNOBL) are critically assessed based on available experimental and theoretical data for phase diagram and thermodynamic properties.

A variety of ternary systems are useful for alloy development with the database. Ternary and binary systems are the building blocks of a CALPHAD assessment.

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.

Calculated phase diagrams of some important ternary systems for noble metal alloys are shown, i.e. Ag-Cu-Zn, Ag-Au-Zn, Au-Cu-Zn, Ag-Au-In, Ag-Au-Cu, Ag-Cu-Ni, Au-Cu-In, Au-Ni-Pt, and Pd-Rh-Ru.

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.

Ag-Cu-Zn

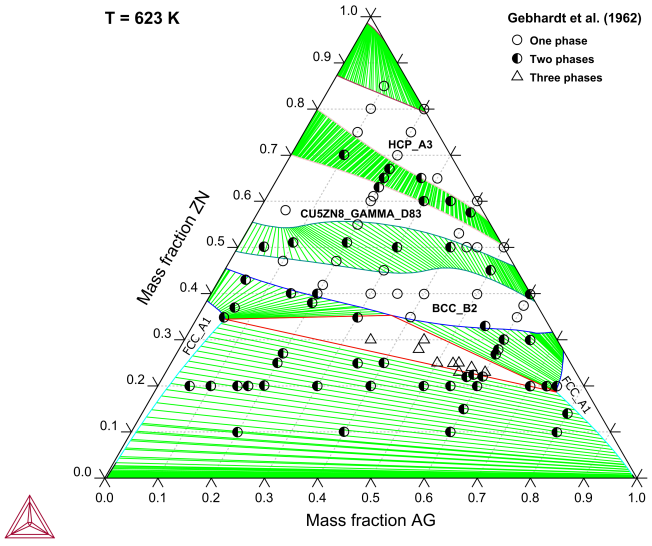

Figure 1: Calculated Ag-Cu-Zn isothermal section at 623 K compared with experimental data [1962Geb].

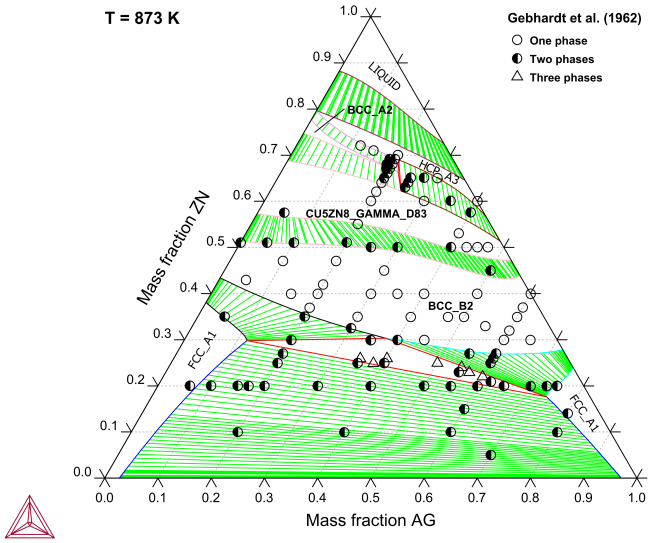

Figure 2: Calculated Ag-Cu-Zn isothermal section at 873 K compared with experimental data [1962Geb].

Ag-Au-Zn

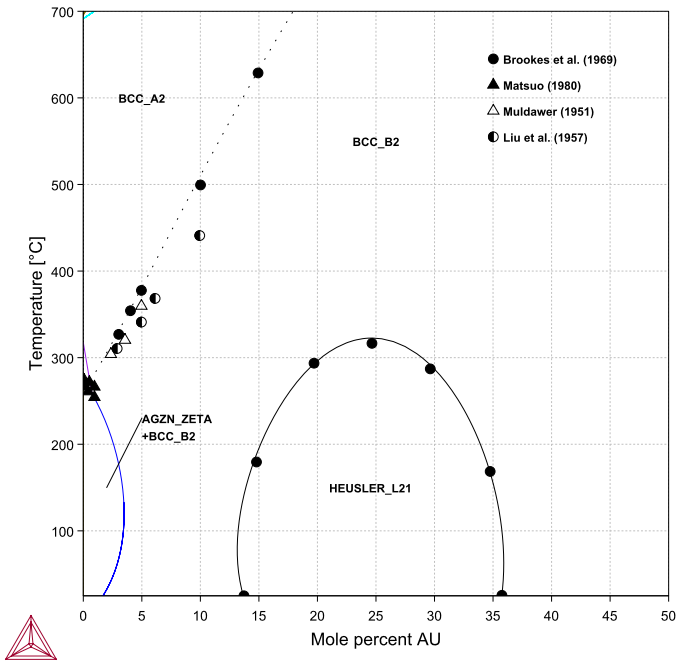

Figure 3: Calculated Ag-Au-Zn vertical section at 50 at. % Zn compared with experimental data [1969Bro; 1980Mat; 1951Mul; 1957Liu].

Au-Cu-Zn

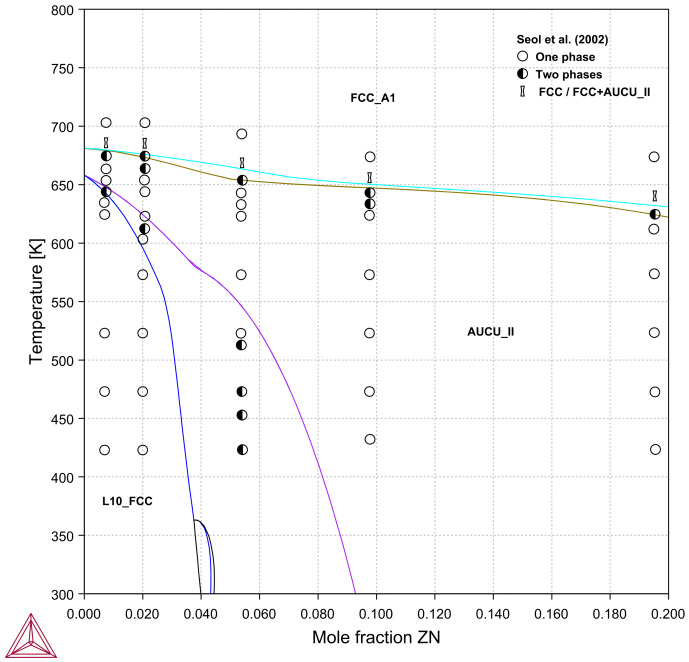

Figure 4: Calculated partial phase diagram for the AuCu-Zn pseudobinary system (up to 20 at.% Zn) compared with experimental data [2002Seo].

Ag-Au-In

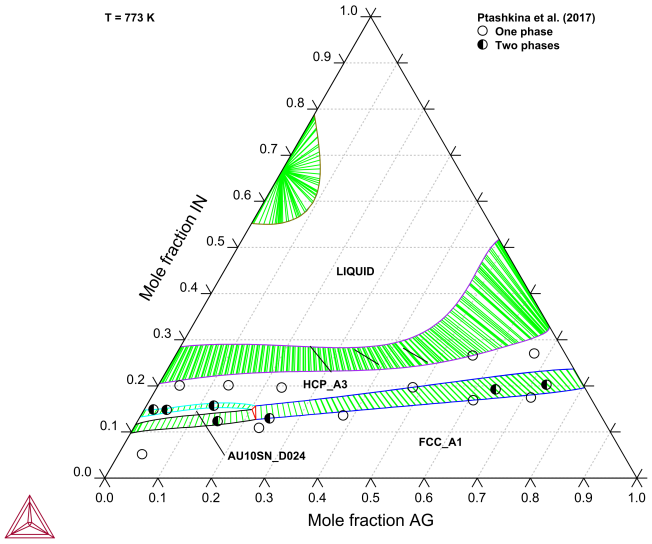

Figure 5: Calculated Ag-Au-In isothermal section at T=773 K compared with experimental data [2017Pta].

Ag-Au-Cu

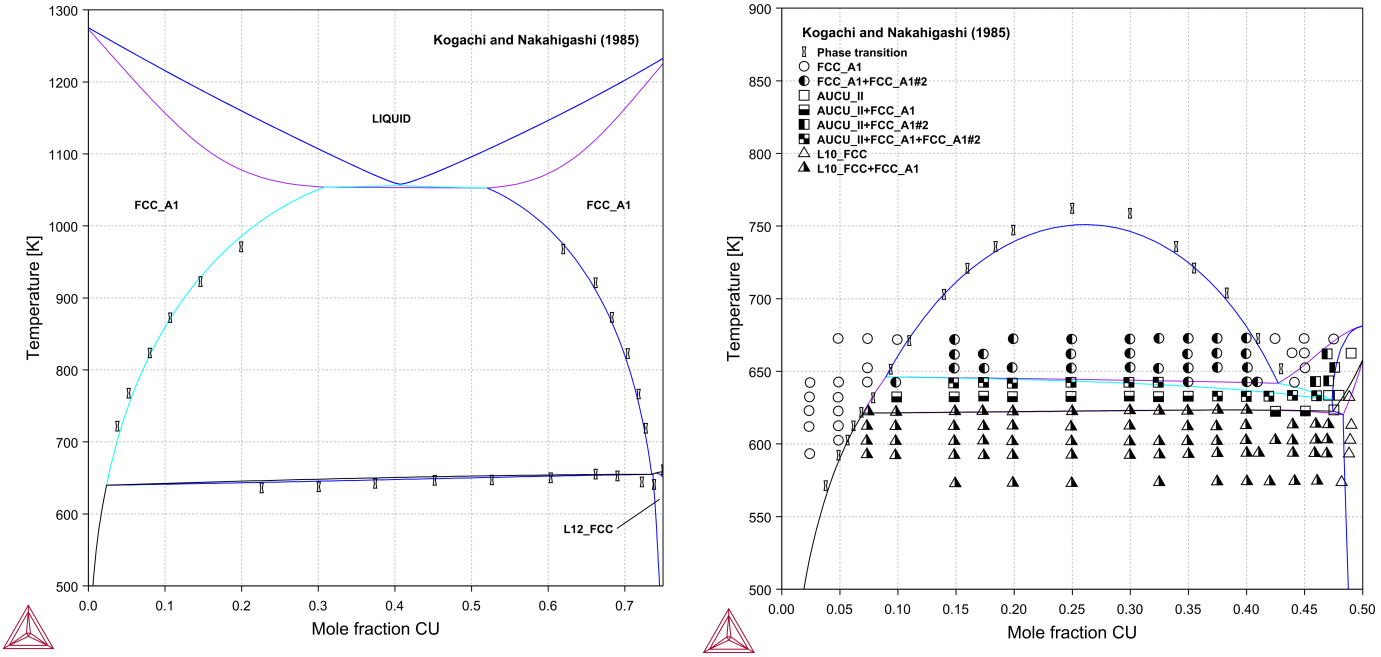

Figure 6: Calculated Ag-Au-Cu vertical section at (left) 25 at. % Au, and (right) 50 at. % Au compared with experimental data [1985Kog].

Ag-Cu-Ni

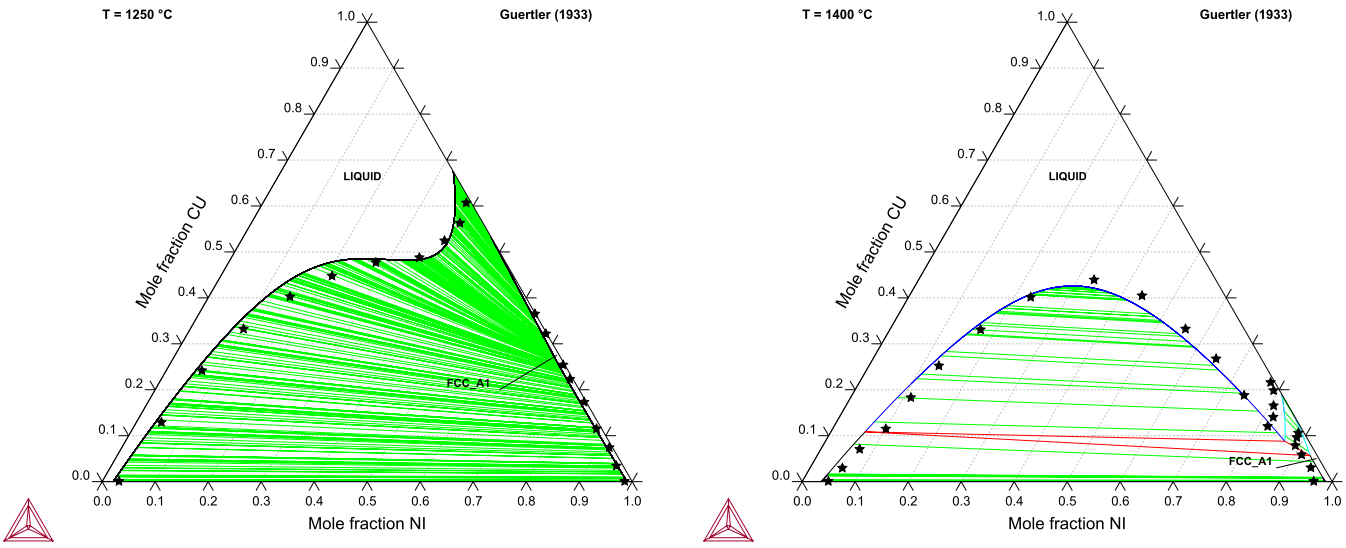

Figure 7: Calculated Ag-Cu-Ni isothermal sections at (left) 1250 °C, and (right) 1400 °C compared with experimental data [1933Gue].

Au-Cu-In

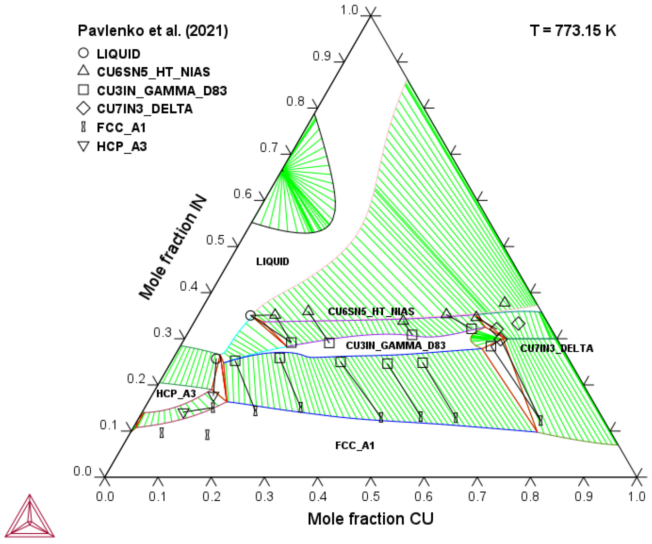

Figure 8: Calculated Au-Cu-In isothermal section at 773.15 K compared with experimental data [2021Pav].

Au-Ni-Pt

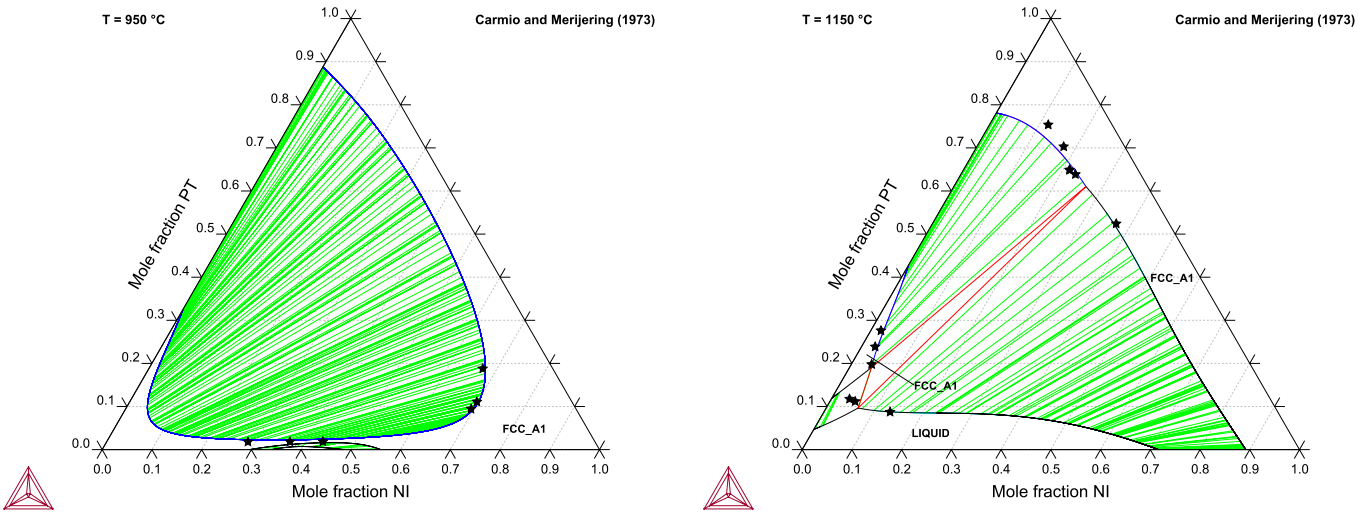

Figure 9: Calculated Au-Ni-Pt isothermal sections at (left) 950 °C, and (right) 1150 °C compared with experimental data [1973Car].

Pd-Rh-Ru

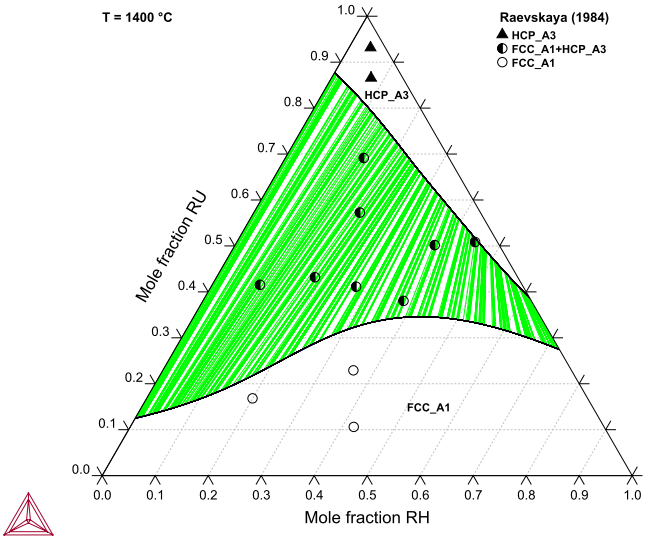

Figure 10: Calculated Pd-Rh-Ru isothermal section at 1400 °C compared with experimental data [1984Rae].

References

[1933Gue] W. Guertler, A. Bergmann, Studies of the Ternary Silver-Copper-Nickel System. Zeitschrift für Met. 25, 53 (1933).

[1962Geb] E. Gebhardt, G. Petzow, W. Krauss, On the Constitution of the Cu-Ag-Zn System. Zeitschrift für Met. 53, 372–379 (1962).

[1969Bro] M. E. Brookes, R. W. Smith, Long range ordering in the system AgAuZn. Scr. Metall. 3, 667–669 (1969).

[1980Mat] Y. Matsuo, The Effect of Additional Elements on the β' → ϵ Transformation in Equiatomic AgZn Alloy. Trans. Japan Inst. Met. 21, 174–178 (1980).

[1951Mul] L. Muldawer, X-Ray Measurement of Long-Range Order in β-AgZn. J. Appl. Phys. 22, 663–665 (1951).

[1957Liu] Y.-H. LIU, C.-C. HSU, An Investigation of Ag-Au-Zn Alloys with 50 AT. % Zn. Acta Phys. Sin. 13, 463–482 (1957).

[1973Car] S.M. Carmio and J.L. Merijering, "The Gold-Nickel- Platinum System," Z.Metall, vol. 64, pp. 170-175, 1973.

[1984Rae] M.V. Raevskaya, V.V. Vasekin, I.G. Sokolova, "The interaction of platinum metals at 1400 °C," J. Less-Common Met., vol. 99, pp. 137-142, 1984.

[1985Kog] M. Kogachi and K. Nakahigashi, "Phase relations in the AuCu1-yAgy and Au(Cu1-yAgy)3 ternary system," Jpn. J. Appl. Phys., vol. 24, pp. 121-125, 1985.

[2002Seo] H.-J. Seol, T. Shiraishi, Y. Tanaka, E. Miura, Y. Takuma, K. Hisatsune, Partial phase diagram for the AuCu–Zn pseudobinary system. J. Alloys Compd. 339, 144–148 (2002).

[2017Pta] E. A. Ptashkina, A. G. Romanova, A. S. Pavlenko, E. G. Kabanova, V. N. Kuznetsov, Phase equilibria in the Ag–Au–In system at 500°C. Russ. J. Phys. Chem. A. 91, 264–267 (2017).

[2021Pav] A. S. Pavlenko, E. A. Ptashkina, G. P. Zhmurko, S. E. Philippova, E. G. Kabanova, V. N. Kuznetsov, Phase equilibria in the Au–Cu–In ternary at 500 °C: Experimental study and CALPHAD modeling. Calphad. 72, 102236 (2021).

Liquidus and Solidus Calculations

For many noble metal products casting is an important part of the production route and some noble metal alloys are even used as solder alloys. For noble metal alloys in other applications it may be of importance to make sure that the designed alloy do not melt at a certain temperature. There are many reasons why it is important to be able to predict the liquidus and solidus temperature as a function of composition for an alloy. Below are two diagrams showing a comparison between calculated and experimental liquidus and solidus temperatures for a large number of commercial noble metal alloys.

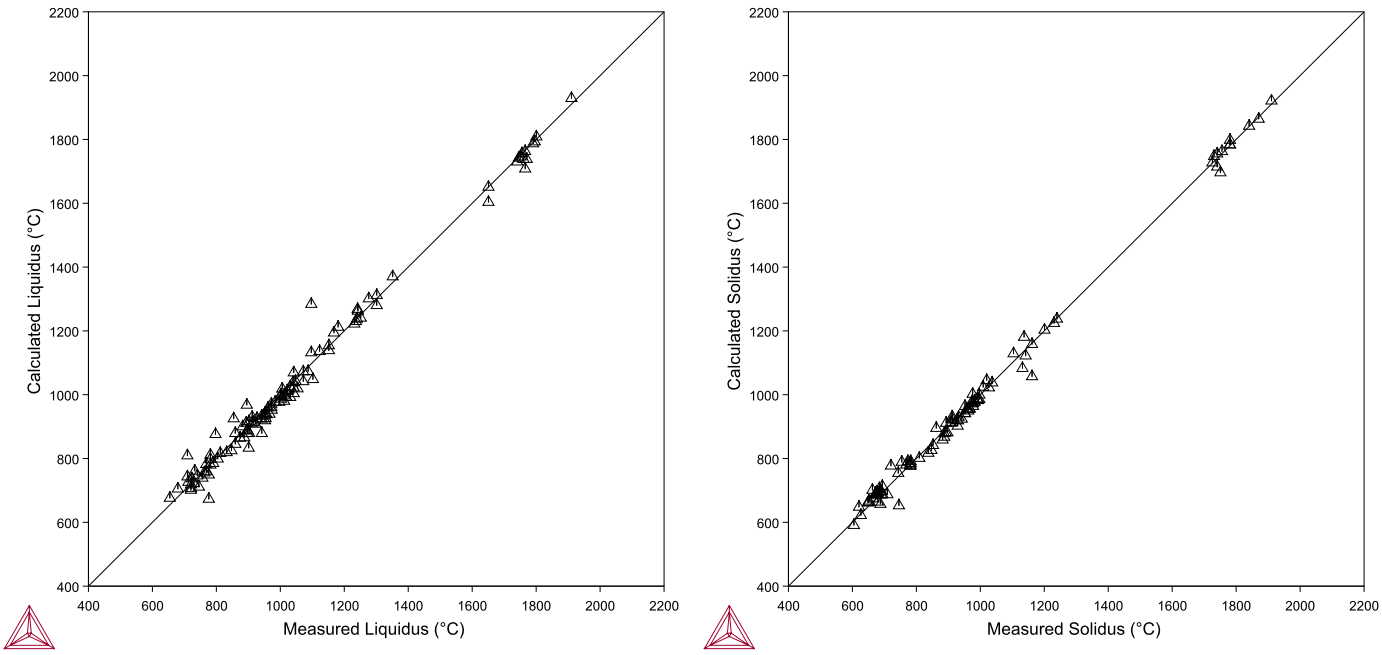

Figure 11: Validation results on (left) liquidus and (right) solidus for a large number of commercial noble metal alloys.

Ag-Cu-Ge

The addition of Ge to Ag-Cu alloys is known to increase both the corrosion resistance and the mechanical properties of the alloy. Due to this the Ag-Cu-Ge ternary system is interesting both for Ag-based solder alloys, but also for sterling silver alloys used for jewelry. The possibility to calculate melting temperature and solidification sequence for alloys in this ternary system is thus important. One example is the calculated liquidus surface projection that shows which solid phase first forms during solidification. Below is the calculated liquidus surface projection for the Ag-Cu-Ge system compared with experimental data [2009Nag; 2015Akh; 2017Guo].

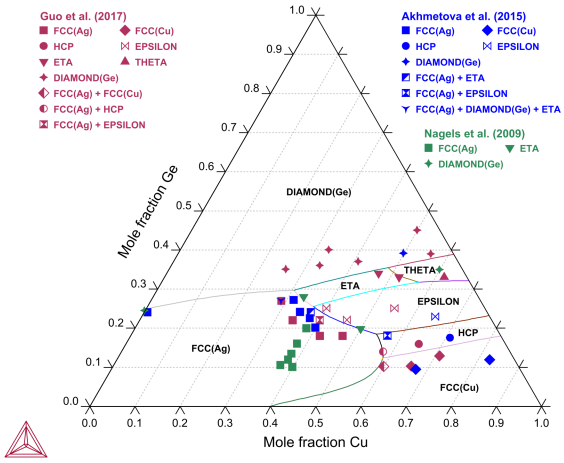

Figure 12: Calculated liquidus surface projection of the Ag-Cu-Ge system in comparison with experimental data [2009Nag; 2015Akh; 2017Guo].

References

[2009Nag] E. Nagels, J. Van Humbeeck, L. Froyen, The Ag–Cu–Ge ternary phase diagram. J. Alloys Compd. 482, 482–486 (2009).

[2015Akh] A. M. Akhmetova, A. T. Dinsdale, A. V Khvan, V. V Cheverikin, A. V Kondratyev, D. O. Ivanov, Experimental investigations of the Ag–Cu–Ge system. J. Alloys Compd. 630, 84–93 (2015).

[2017Guo] C. Guo, L. Zou, C. Li, Z. Du, Experimental Investigation and Thermodynamic Modeling of the Ag-Cu-Ge System. Metall. Mater. Trans. A. 48, 4965–4976 (2017).

Solidification and Homogenization in the Diffusion Module (DICTRA)

The following examples are predicted using the Diffusion Module (DICTRA), with a combination of TCS Noble Metal Alloys Database (TCNOBL) and TCS Noble Metal Alloys Mobility Database (MOBNOBL).

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.

Homogenization of Alloys

In this example, the concentration profiles in Au/Au-Fe and Fe/Pd-Fe diffusion couples at different times and temperatures.

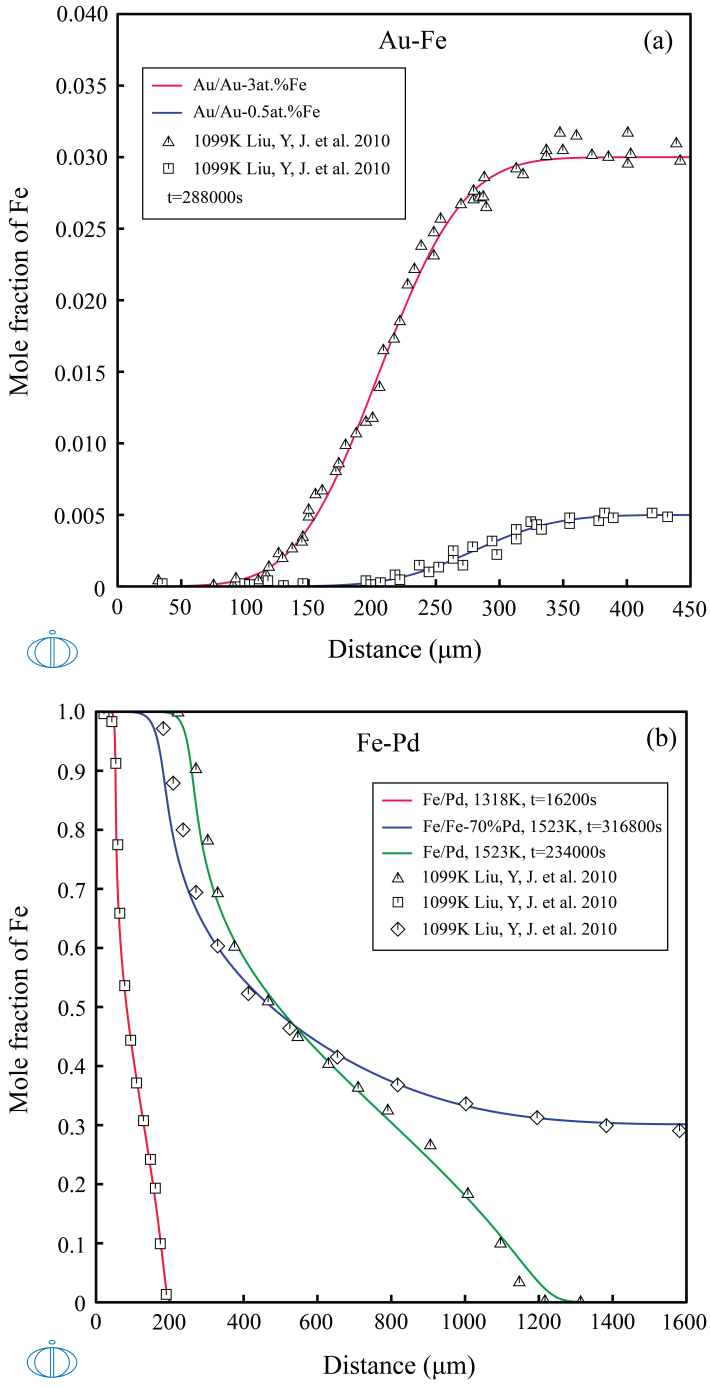

Figure 13: The calculated concentration profiles in the (top labeled A) Au/Au-Fe and (bottom labeled B) Fe/Fe-Pd diffusion couples as a function of time and temperatures, compared with experimental data [2010Liu].

Simulation of Isothermal Solidification

Similar to other alloys, solidification is also one of the most critical processes in noble metal alloys. Being able to accurately simulate the solidification behaviors of a noble metal alloy is of great importance.

With solidification simulations, the evolution of phase fraction, the position of phase boundary, and so forth as a function of time and temperature can be predicted .

Transient liquid phase (TLP) bonding or diffusion brazing is a bonding process that has been developed to join materials which are otherwise very difficult to join. The bonding process is a brazing or soldering variation that utilizes an interlayer that melts at a temperature lower than that of the substrate to form a liquid at the faying surface. Due to the facts that 1) the TLP bonding is controlled by the diffusion of the solutes into the solid solvent that takes time on the order of hours; 2) designing a TLP process is time-consuming, and the examining results of estimating the width of the remaining eutectic liquid from the solidified joint cross sections may easily remain errors. Therefore, quantitatively and accurately predict the solid/liquid interface kinetics during the isothermal solidification stage of TLP bonding in an noble metal alloy is of great importance.

In this example, the phase transitions of Ag-43at.%Cu-14at.%Au during the isothermal solidification was predicted. The width of the liquid phase layer starts to increase in the beginning due to the change in solidus/liquidus composition and mass balance requirements, once the maximum liquid width has been reached, the solutes will diffuse into the base metal and the fraction of liquid phase starts to decrease.

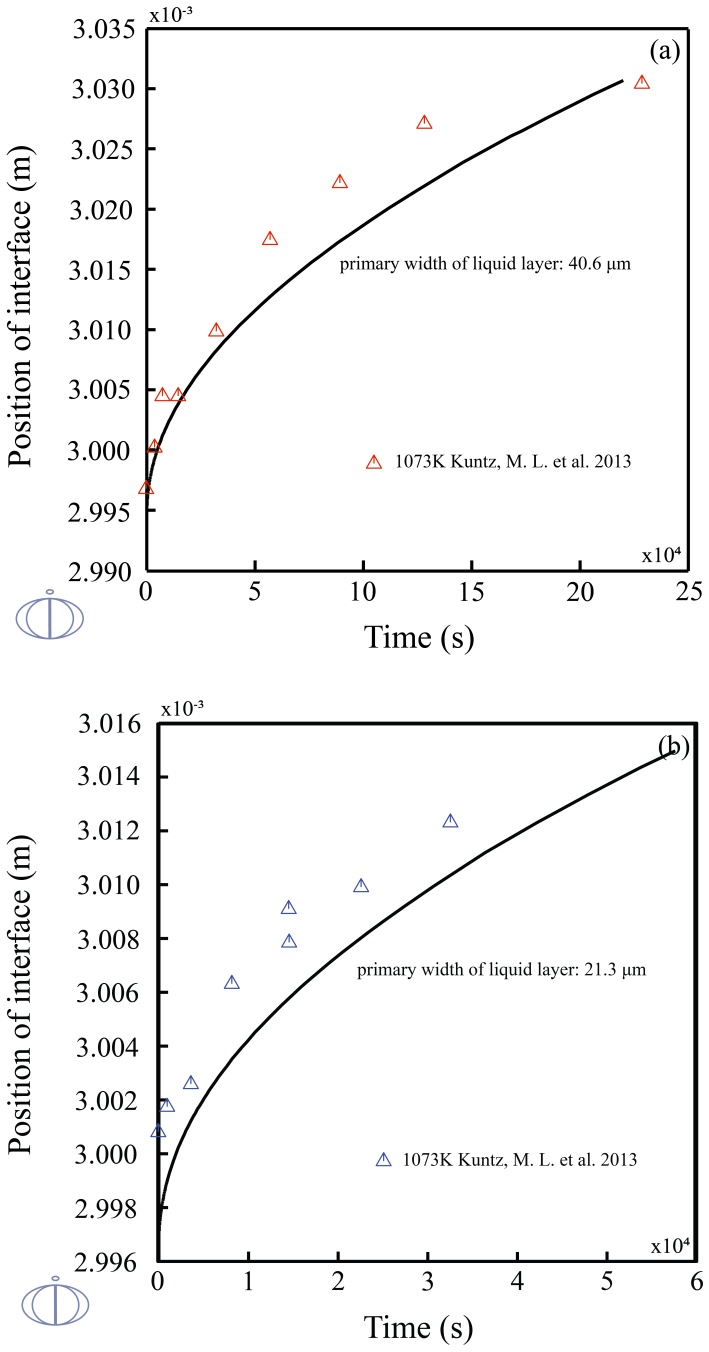

Figure 14: The calculated positions of interface vs. time at 1073K in the diffusion couples of the (solid) pure Ag/ (liquid)Ag-43at.%Cu-14at.%Au with the primary widths of liquid layer (top labeled A) 40.6 µm and (bottom labeled B) 21.3 µm along with the experimental data [2013Kun].

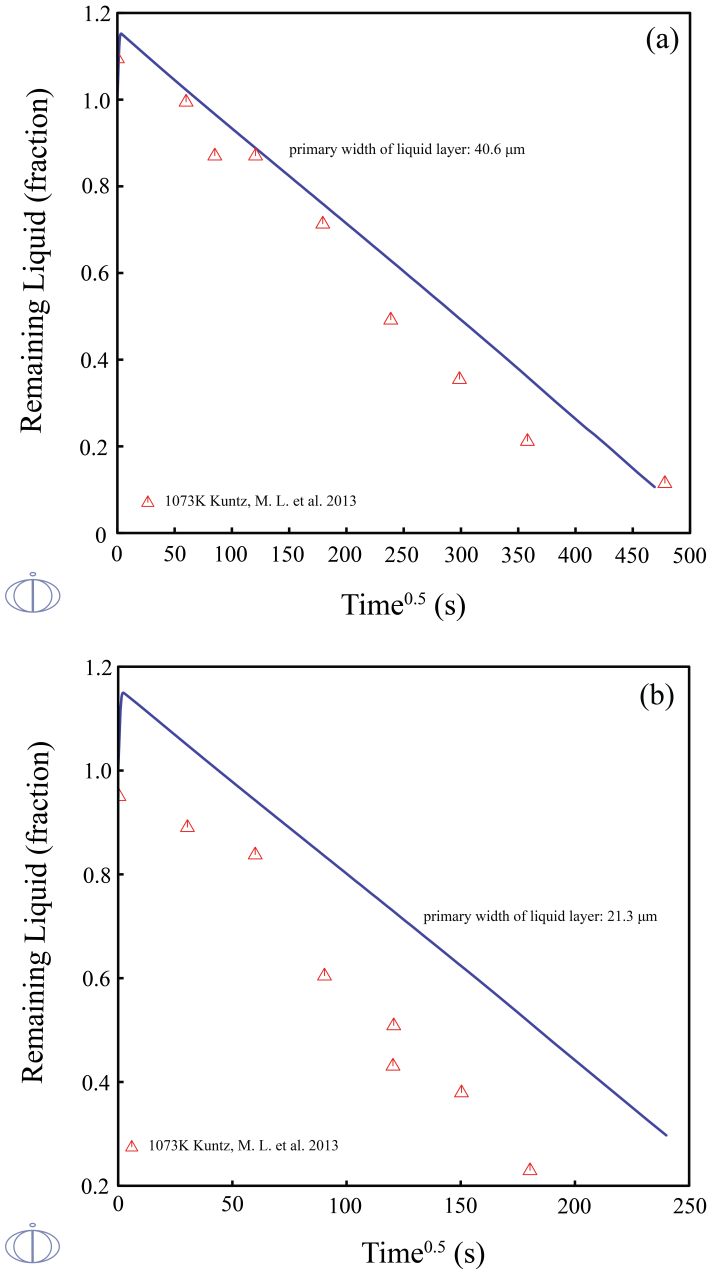

Figure 15: The calculated fraction of remaining liquid vs. time at 1073K in the diffusion couples of the (solid) pure Ag/ (liquid)Ag-43at.%Cu-14at.%Au with the primary widths of liquid layer (top labeled A) 40.6 µm and (bottom labeled B) 21.3 µm along with the experimental data [2013Kun].

References

[2010Liu] Y. Liu, J. Wang, Y. Du, L. Zhang, D. Liang, Mobilities and diffusivities in fcc Fe–X (X=Ag, Au, Cu, Pd and Pt) alloys. Calphad. 34, 253–262 (2010).

[2013Kun] M. L. Kuntz, B. Panton, S. Wasiur-Rahman, Y. Zhou, S. F. Corbin, An Experimental Study of Transient Liquid Phase Bonding of the Ternary Ag-Au-Cu System Using Differential Scanning Calorimetry. Metall. Mater. Trans. A. 44, 3708–3720 (2013).

Precipitation Analysis of an Au-Co Alloy

Volume fractions of the precipitated phase and TTT diagrams of heat treatment have a decisive influence on the subsequent mechanical properties of high-strength precipitation-hardened noble metal alloys.

These calculations are well represented using the Precipitation Module (TC-PRISMA) with a combination of TCS Noble Metal Alloys Database (TCNOBL) and TCS Noble Metal Alloys Mobility Database (MOBNOBL), which are used in the following examples.

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.

The Au-Co alloy system has been proposed as dental casting gold alloy due to its precipitation phenomenon of age-hardening process. In this example, the precipitation and TTT diagrams were simulated in the Au-1wt.%Co, from which a hcp or fcc (Co-riched) phase precipitates in the fcc-Au matrix. The criterion of determining the largest hardness in [1976Miy] is

$$log_{10}[-ln(1-f)] = 0$$

where f is the transformed fraction of the precipitating process, ranging from 0 to 1. According to the criterion, the value of f with the largest hardness is 0.6321. The volume fractions of precipitates changing with time can then be predicted by multiplying the largest volume fraction by f. Therefore, the stop criterion of volume fraction in our simulation was chosen as the value obtained by multiplying the largest volume fractions and 0.6321. Furthermore, the mobility enhancement parameters and dislocation densities were applied due to the existence of dislocations. The parameters and the dislocation densities were derived by the apparent diffusivities of FCC_A1 Au-Co alloys. The input parameters for simulations are listed in the table, and the simulated results are shown in the plots below.

The input parameters for simulations.

		Mobility Adjustment		*Dislocation Densities*
		Prefactor	Q	1wt%Co
Precipitate	FCC	2.2	-1414.0143	5.288e13/m2
	HCP	18	-1414.0143	5.288e13/m2

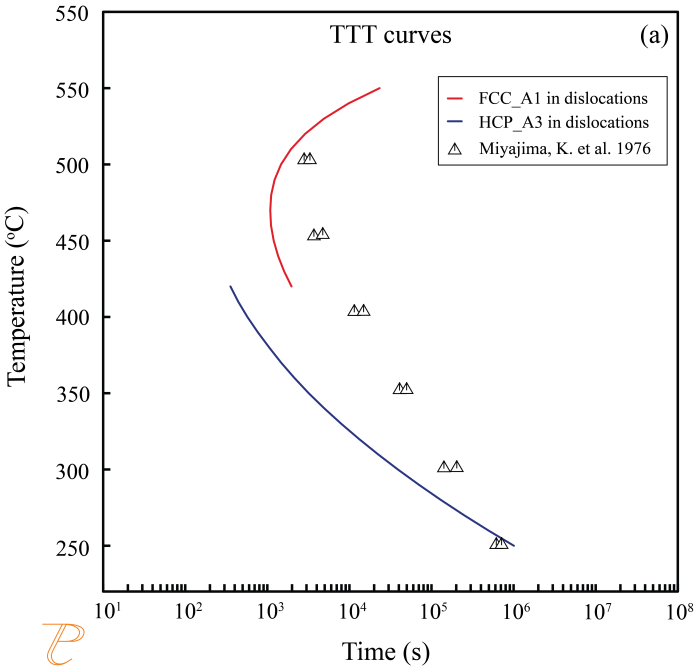

Figure 16: Simulated TTT curves of the precipitated hcp and fcc phases in the Au-1wt.%Co alloy with aging time at different temperatures, compared with the experimental data from [1976Miy].

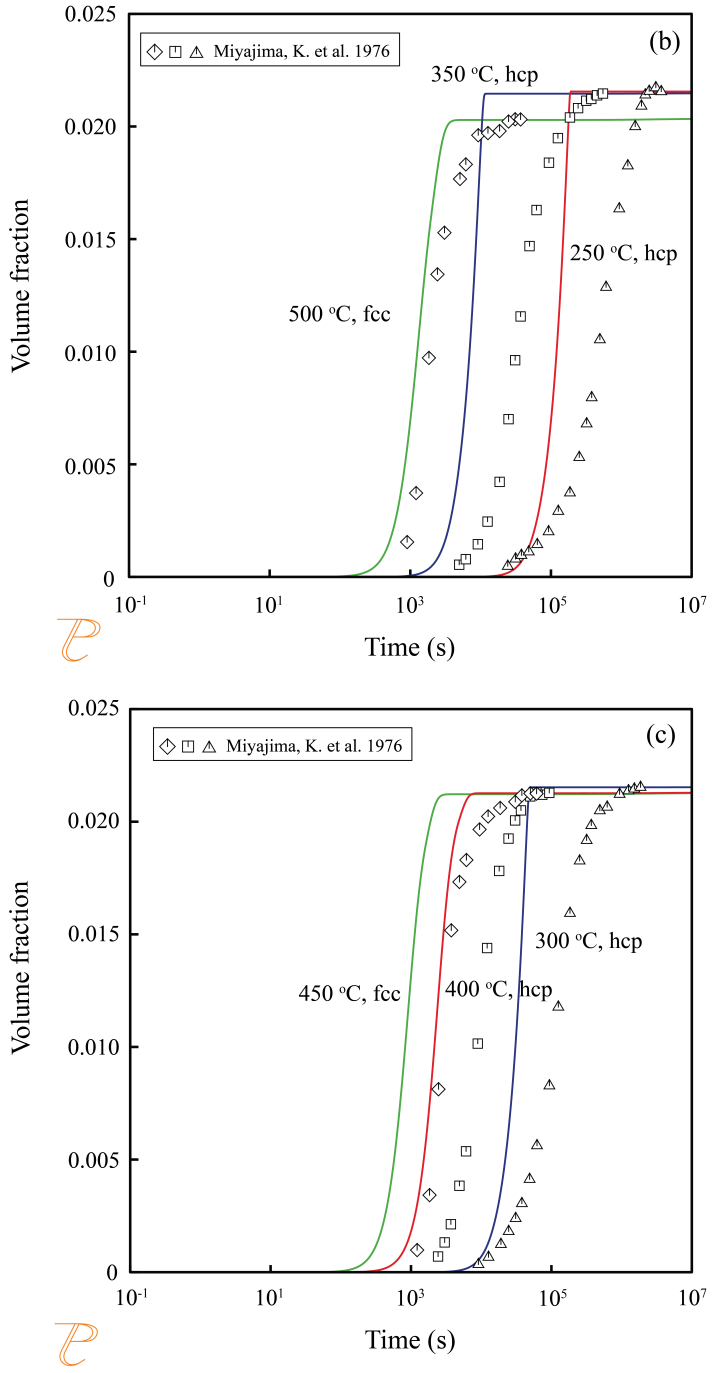

Figure 17: Volume fractions of the precipitated hcp (top labeled B) and fcc (bottom labeled C) phases in the Au-1wt.%Co alloy with aging time at different temperatures, compared with the experimental data from [1976Miy].

Reference

[1976Miy] Y. MIYAJIMA, K. YASUDA, Y. KANZAWA, Precipitation Hardening in Gold-Cobalt Alloys. Bull. Tokyo Med. Dent. Univ. 23, 41–51 (1976).

TCNOBL Surface Tension and Density of Ag-Au-Cu

One of the most important ternary systems for noble metal alloys is Ag-Au-Cu and this ternary system is used as an example to calculate the surface tension and density of liquid.

The surface tension thermophysical property data is included with the TCS Noble Metal Alloys Database (TCNOBL) as of version 3 (TCNOBL3).

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-Au-Cu

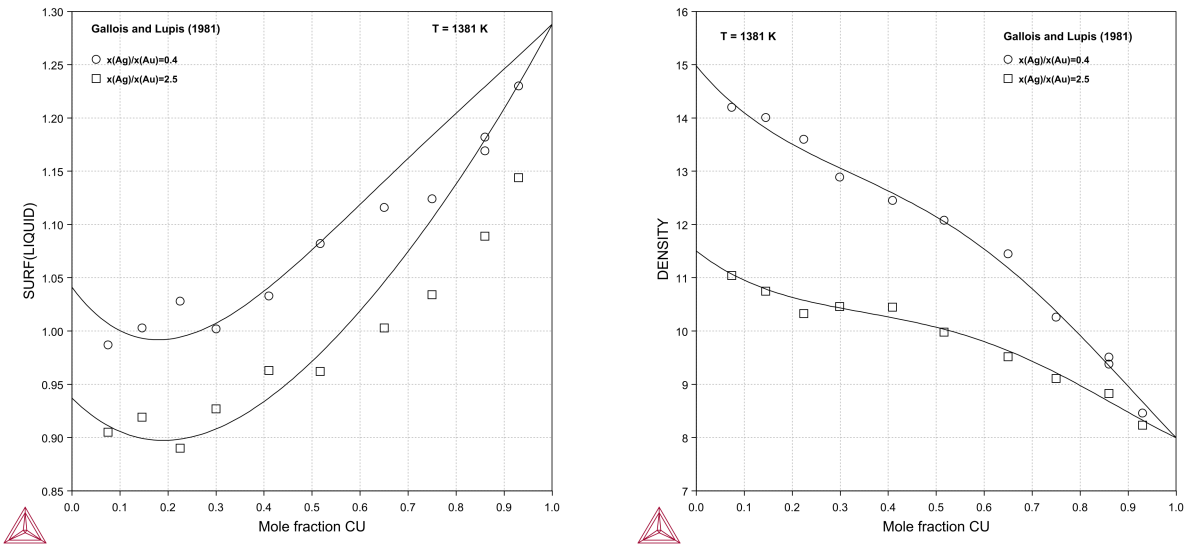

Figure 18: Calculated surface tension (left) and density (right) of liquid for Ag-Au-Cu alloys with x(Ag)/x(Au)=0.4 and x(Ag)/x(Au)=2.5 compared with experimental data [1981Gal].

Reference

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

TCNOBL Viscosity Example

The viscosity thermophysical property data is included with the TCS Noble Metal Alloys Database (TCNOBL) starting with version 3 (TCNOBL3).

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.

One of the most important ternary systems for noble metal alloys is Ag-Au-Cu and this ternary system is used as example for calculation of dynamic viscosity of liquid.

Ag-Au-Cu

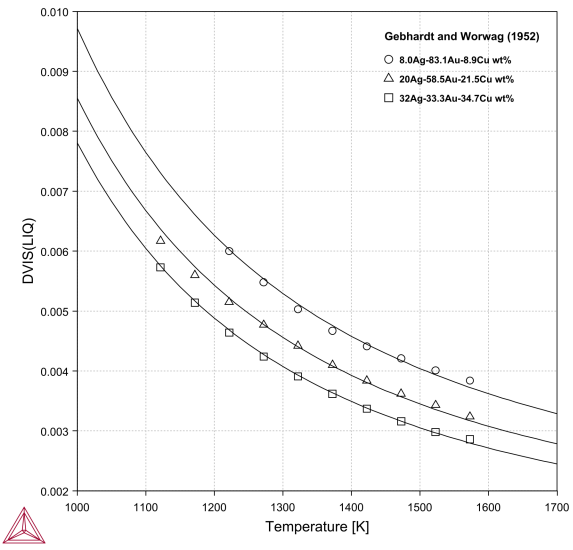

Figure 19: Calculated dynamic viscosity of liquid for three different Ag-Au-Cu alloys compared with experimental data [1952Geb].

References

[1952Geb] E. Gebhardt, G. Worwag, Die innere Reibung flüssiger Legierungen ans Silber-Kupfer-Gold. Zeitschrift für Met. (International J. Mater. Res.) 43, 106–108 (1952).

TCNOBL Electrical Resistivity Examples

Electrical resistivity (ELRS) of noble metal alloys can be calculated using Thermo-Calc and with the TCS Noble Metal Alloys Database (TCNOBL). 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 3.0 (TCNOBL3).

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.

In these validation examples, calculated ELRS values are compared with experimental data for some noble metal alloys. In some of the examples the experiments are performed on "frozen-in" structures, i.e. the structure consists of only a single disordered FCC phase. In other experiments the samples are heat treated for a longer time and can be considered to have reached equilibrium. The comparison calculations are carried out in accordance with the corresponding experiments.

Ag-Au-Cu

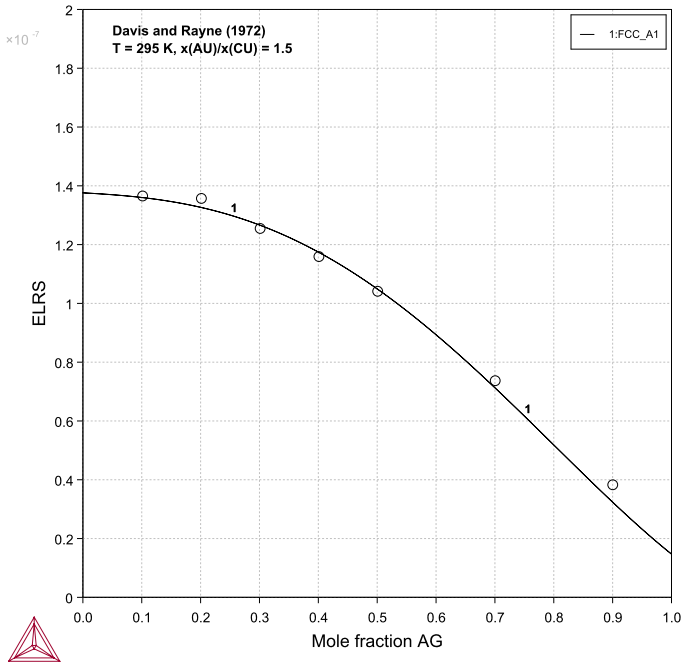

Figure 20: Calculated electrical resistivity of disordered (frozen-in FCC structure) Ag-Au-Cu alloys at 295 K compared with experimental data [1972Dav].

Au-Cu-Zn

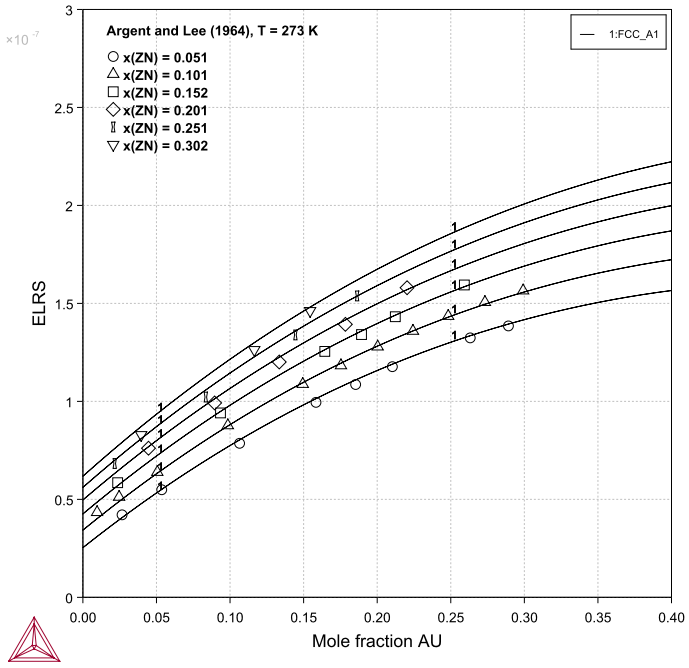

Figure 21: Calculated electrical resistivity of disordered (frozen-in FCC structure) Au-Cu-Zn alloys at 273 K compared with experimental data [1964Arg].

Ag-In-Sn

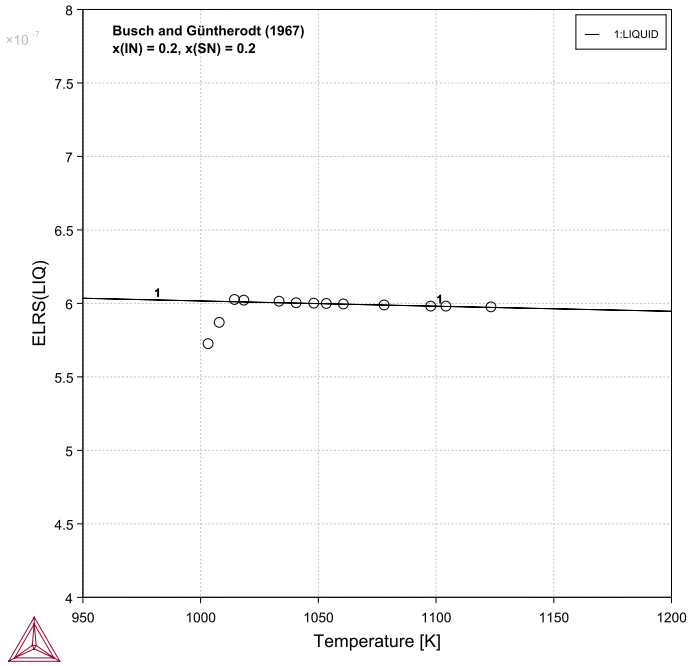

Figure 22: Calculated electrical resistivity of liquid for an Ag-In-Sn alloy with 20 at% In and 20 at% Sn compared with experimental data [1967Bus].

Ag-Cu-Pd

In experiments by Volkov [2004Vol], samples of a Cu-Pd-10Ag alloy are first heat treated at 850 °C and then quenched. This results in a material with a "frozen-in" single phase FCC structure. Electrical resistivity was then measured as a function of time during isothermal heat treatment at 370 °C. At the end of the measurement it can then be assumed that equilibrium was reached. The diagram shows calculated electrical resistivity compared with the measured results by Volkov [2004Vol], both for the initial state and at equilibrium.

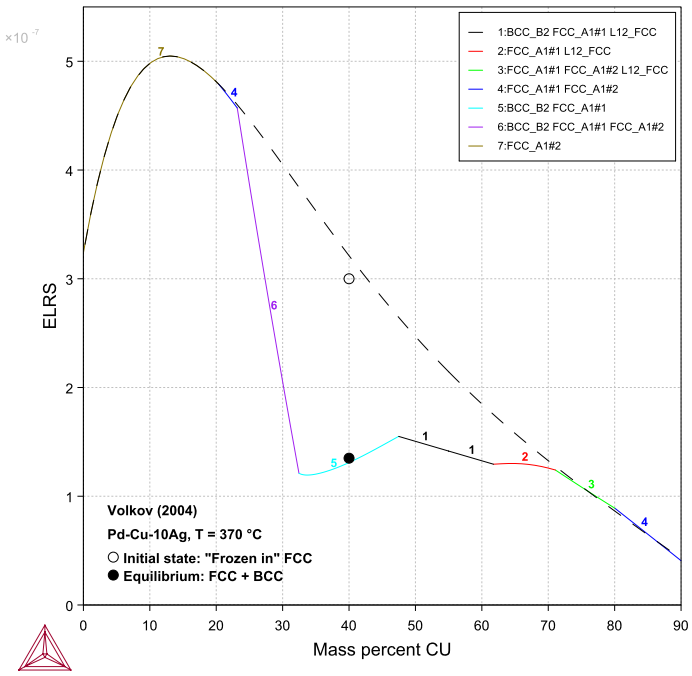

Figure 23: Calculated electrical resistivity of a Cu-Pd-10Ag alloy at 370 °C as a function of composition. The dashed line is the calculated initial state, i.e. a "frozen-in" FCC structure. Colored lines are the calculated equilibrium state. Calculated results are compared with experimental data [2004Vol].

References

[1964Arg] B. B. Argent and K. T. Lee, The electrical resistivities and lattice parameters of copper-gold-zinc alloys, Br. J. Appl. Phys. 15, 1523, (1964).

[1967Bus] G. Busch and H. -J. Güntherodt, Hall-Koeffizient und spezifischer elektrischer Widerstand flüssiger Metallegierungen, Physik der kondensierten Materie volume 6, 325–362 (1967).

[1972Dav] T. H. Davis and J. A. Rayne, Specific Heat and Residual Resistivity of Binary and Ternary Noble-Metal Alloys, Phys. Rev. B, 6, 2931 (1972).

[2004Vol] A. Y. Volkov, Improvements to the Microstructure and Physical Properties of Pd-Cu-Ag Alloys, Platinum Metals Rev., 48, (1), 2, (2004).

TCNOBL 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 Noble Metal Alloys Database (TCNOBL) are critically assessed based on available experimental and theoretical data for phase diagram and thermodynamic properties.

Some important key binary systems for noble metal alloys are shown here, for example, Au-Cu, Ag-Pt, Cu-Pd, Ag-Zn, Mn-Pd, and Mn-Pt 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.

Au-Cu

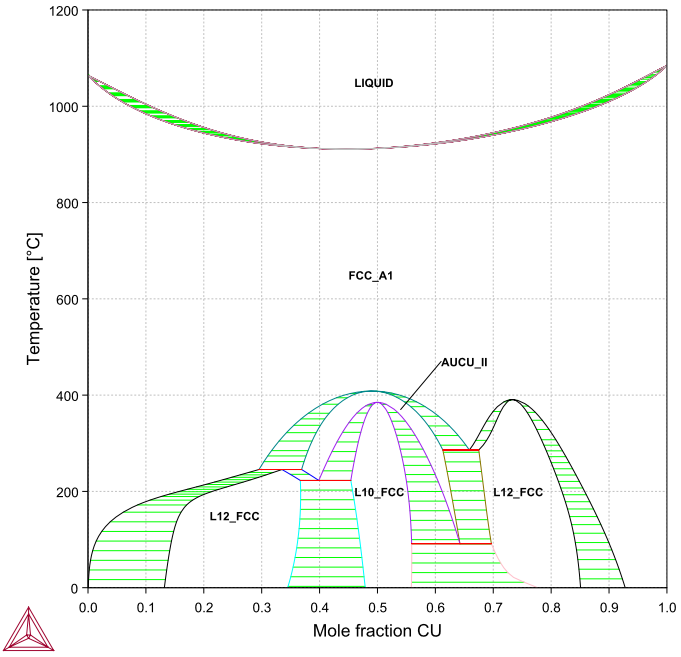

Figure 24: Calculated Au-Cu phase diagram.

Ag-Pt

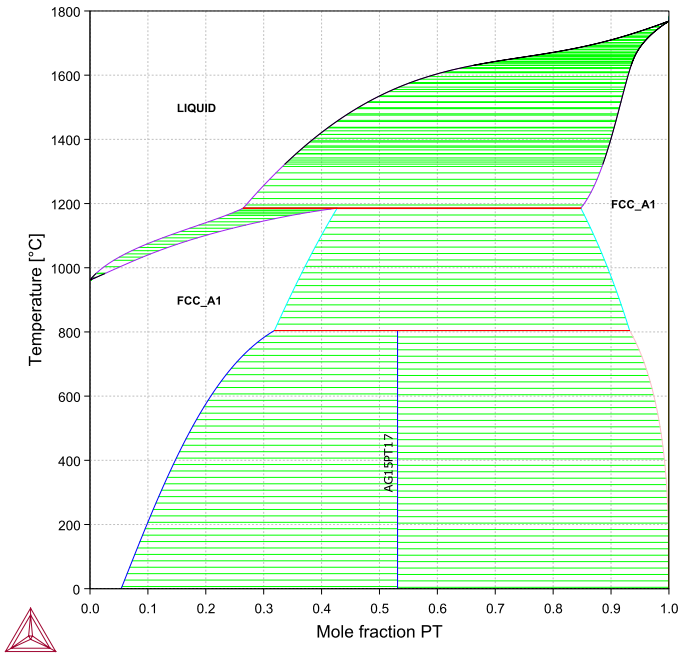

Figure 25: Calculated Ag-Pt phase diagram.

Cu-Pd

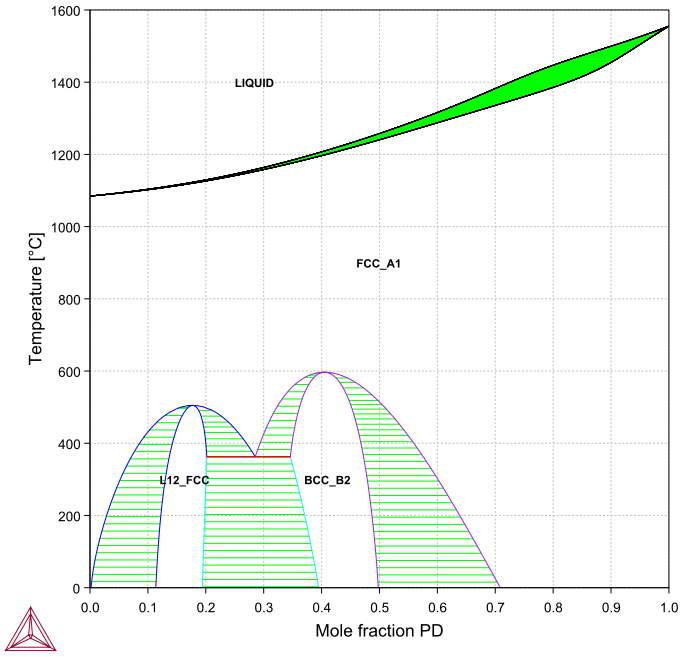

Figure 26: Calculated Cu-Pd phase diagram.

Ag-Zn

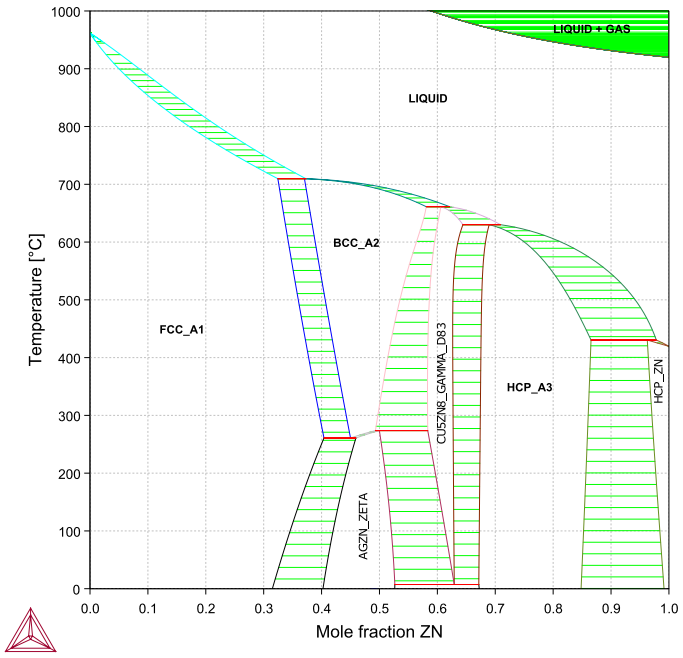

Figure 27: Calculated Ag-Zn phase diagram. Description by Gómez-Acebo [1998Góm] but with modified CU5ZN8_GAMMA_D83.

Mn-Pd

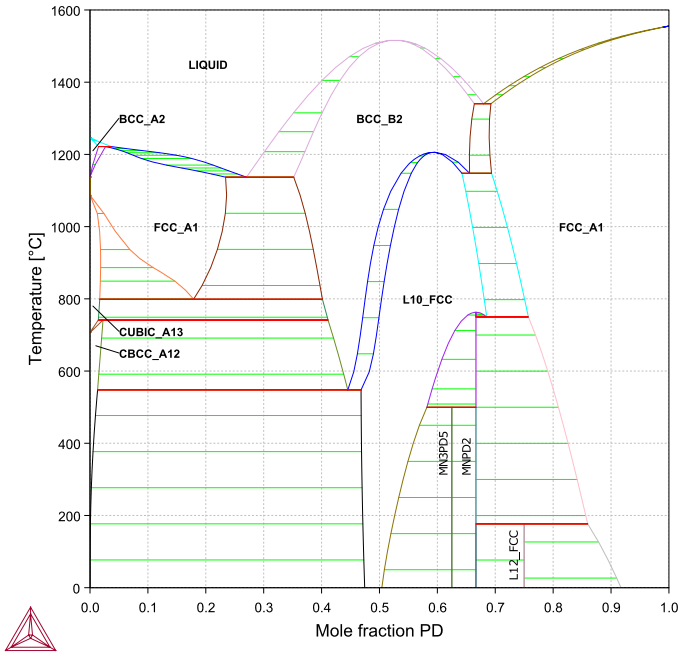

Figure 28: Calculated Mn-Pd phase diagram.

Mn-Pt

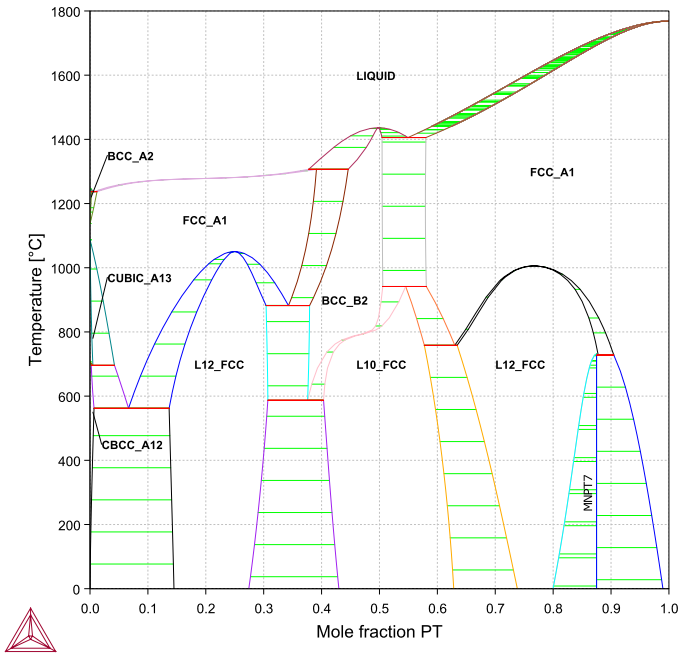

Figure 29: Calculated Mn-Pt phase diagram.

Reference

[1998Góm] T. Gómez-Acebo, Thermodynamic assessment of the Ag-Zn system. Calphad. 22, 203–220 (1998).