

# **TCS Noble Metals Mobility Database (MOBNOBL1)**

## **Technical Information**

Available Starting with Thermo-Calc Version 2022a



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## **MOBNOBL1: TCS Noble Metal Alloys Mobility Database**

TCS Noble Metal Alloys Mobility Database (MOBNOBL) is a kinetic database containing mobility data for noble metal alloys. It can be used for the atomic mobility descriptions of Ag-Au-Cu-Pd-Pt-based alloys for the fcc and liquid phases.

MOBNOBL1 is intended for use in combination with the TCNOBL1 TCS Noble Metal Alloys thermodynamic database.

Together with the Diffusion Module (DICTRA) and a thermodynamic database for noble metals, it can be used to study diffusion-controlled phenomena in noble metals e.g. microsegregation during solidification, homogenization kinetics, growth/dissolution kinetics of precipitates, interdiffusion, and so forth. You can also use it with the Precipitation Module (TC-PRISMA) to simulate concurrent nucleation, growth, and coarsening of precipitates in noble metal alloys.

## **Included Elements (21)**

| Ag | Al | Au | Со | Cr | Cu | Fe | Ga | Ge | In | Ir |
|----|----|----|----|----|----|----|----|----|----|----|
| Mn | Ni | Pd | Pt | Re | Rh | Ru | Sn | Ti | Zn |    |

### **Included Phases**

FCC A1 and LIQUID.



The above phases have diffusion data included in the database. You can include other phases in a diffusion simulation. However, these other phases are treated as so-called diffusion *NONE*, i.e. there is no diffusion considered in these other phases. Any phase not listed above is automatically entered as diffusion *NONE* (in Console Mode in the DICTRA module or in Graphical Mode with the Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA)), as long as a thermodynamic description for the phases is retrieved prior to reading data from the mobility database.

## **Assessed Systems**

All data sets are critically assessed against experimental information whenever available. The fact that the amount of experimental diffusion data is limited for noble metal alloys has made it necessary to use abinitio calculations and sound empirical rules extensively in the development of this kinetic database.

#### FCC\_A1

The database contains assessed/ab-initio calculated/empirically predicted impurity diffusion data in Ag, Au, Cu, Pd, and Pt for all 21 elements. Complete and critical assessments for FCC\_A1 in 27 binary systems and three ternary systems are also included.

### LIQUID

Data for diffusion in liquid Ag, Au, Cu, Pd, and Pt are also assessed or estimated for all 21 elements in the database. Complete and critical assessments of four binary systems for the liquid phase are included.

#### Limits

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

#### **Additional Resources**



Go to the <u>Noble Metal Alloys Databases</u> page on our website where you can access technical information and learn more about its compatible thermodynamic database. Also explore further <u>applications of Thermo-Calc to Precious Metals</u> including links to other resources such as publications and examples.



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