

TCS Zr-based Alloys Mobility Database (MOBZR1)

Technical Information

Available Starting with Thermo-Calc Version 2023a



Contents

MOBZR1: TCS Zr-based Alloys Mobility Database	3
Included Elements	3
Included Phases	3
Assessed Systems	3
Limits	4
Additional Resources	4

MOBZR1: TCS Zr-based Alloys Mobility Database

TCS Zr-alloys Mobility Database (MOBZR) is a kinetic database containing mobility data for Zr-based alloys. Data is present in a format suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA), and/or for use together with any Thermo-Calc programming interface such as TC-Python or TC-Toolbox for MATLAB®.

MOBZR1 is intended for use in combination with the TCZR1 (TCS Zr-based Alloys) thermodynamic database.

Together these databases can be used with the Diffusion Module (DICTRA) to study diffusion-controlled phenomena in zirconium alloys, e.g. microsegregation during solidification, homogenization kinetics, growth/dissolution kinetics of precipitates, interdiffusion, and so forth. You can also use the databases with the Precipitation Module (TC-PRISMA) to simulate concurrent nucleation, growth, and coarsening of precipitates in Zr-based alloys.

Included Elements

There are eight (8) elements included in the current version of the database.

Cr	Fe	H	Nb	Ni	O	Sn	Zr
----	----	---	----	----	---	----	----

Included Phases

BCC_A2, HCP_A3, and LIQUID



The 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

The BCC_A2 and HCP_A3 systems are assessed.

The unary systems and some of the binaries (Cr-Fe, Cr-Ni, Cr-H, Fe-H, Fe-Ni, Fe-O, Nb-H) already exist in the other mobility databases. The mobility parameters were tested for compatibility and combined with the assessments.

Mobility parameters for the Zr-Cr, Zr-Fe, Zr-H, Zr-Nb, Zr-Ni, Zr-O, and Zr-Sn systems are assessed.

Limits

The database is applicable for most commercial Zr-based alloys; care should be taken with alloys including high amounts of alloying elements.

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 [Zirconium-based Alloys Database](#) page on our website where you can access an examples collection and the technical information.



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