TCS Zr-based Alloys Database (TCZR1)

Technical Information

Available Starting with Thermo-Calc Version 2022a

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Contents

About the TCS Zr-based Alloys Database (TCZR)

The TCS Zr-based Alloys Database (TCZR) is a thermodynamic and properties database for zirconium-based alloys. It can be used for a wide range of compositions from pure zirconium to complex zirconium-based commercial zirconium alloys. It can be used for calculating phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria and simulating solidification processes for a wide range of zirconium alloys of industrial relevance, including but not limited to:

- Nuclear-grade zirconium alloys
- Experimental zirconium alloys under development

The current version of the database is TCZR1.

In addition to thermodynamic data, it has thermophysical properties data available for:

- Molar volume and thermal expansivity of all solid phases and liquid
- Viscosity of liquid
- Surface tension of liquid

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 binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

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

Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application areas such as process metallurgy, heat treatment, and more depending on the database. Sometimes an example is both a validation and a calculation example.

Some use case examples of how this database can be used include the following. Use it to enable predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulation and

Scheil solidification simulations) to be made for multicomponent systems and alloys of industrial importance. This means that the database can be used to extrapolate to higher-order systems by combining several critically assessed systems.

Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at info@thermocalc.com. The experts are available to make recommendations on the most suitable database to use for your needs.

TCS Zr-based Alloys Database (TCZR) 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 Zr-based Alloys Database (TCZR) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, and the phases and models. It also includes a list of the included elements and general information about the included thermophysical properties data.
- The *TCS Zr-based Alloys Database (TCZR) 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 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.

TCZR1 Elements, Systems, Phases and Properties

Included Elements

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

Cr	Fe	H	Nb	Ni	O	Sn	Zr

Assessed Systems and Phases

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling have been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges.

All the stable solution phases and intermetallic compounds that exist in each assessed system are included. Note that in most cases phases having the same crystal structure had been merged as the same phase.

The current version of the database contains:

- 28 assessed binary systems
- 19 assessed ternary systems
- 69 phases

In Console Mode, you can list phases and constituents in the Database (TDB) module and the Gibbs (GES) module. For some phases, supplementary information is included in the definitions. To show the information, it is recommended in the Database (TDB) module to use the command LIST_SYSTEM with the option `Constituents`.

Properties Data

A variety of properties data is included with the TCS Zr-based Alloys Database (TCZR).

- In total, 28 binary systems have viscosity parameters for the liquid phase.
- 28 binary systems have surface tension parameters for the liquid phase.
- Volume parameters have either been assessed or estimated for all solid phases and for the liquid phase. Interactions have been either assessed or estimated for every binary combination in the common solution phases, including liquid, fcc_A1, bcc_A2 and hcp_A3.

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 thermophysical 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.

Below is a summary of the available parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the online help.

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Surface tension	SIGM, XI	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)`
Kinematic viscosity		`KVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

TCZR1 Systems

In this section:

TCZR1 Assessed Binary Systems

These are the assessed binary systems in the full range of composition and temperature.

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

TCZR1 Assessed Ternary Systems

These are the assessed ternary systems.

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

TCZR1 Phases

In this section:

Common Phases for Zirconium Alloys

TCZR1 Models for the Included Phases

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key zirconium alloys.

Name in the Database	*Common Name and Description*
LIQUID	Liquid phase, which covers the melt of Zr alloys
BCC_A2	β zirconium, Bcc type solid solution phase, which covers the high temperature (Zr) matrix phase
HCP_A3	α zirconium, Hcp type solid solution phase, which covers the low temperature (Zr) matrix phase
C14_Laves	Laves_C14 phase, which covers some Zr/Nb-compounds, high temperature Cr_2Zr, Fe_2Nb
C15_Laves	Laves_C15 phase, which covers some Zr-compounds, Cr_2Zr, Fe_2Zr etc.
C16_Theta	Laves_C36 phase, which covers $MgNi_2$, $(Cu,Zn)_2Mg$ and $(Al,Mg)_2Ca$
FeNbZr_τ	$(Zr,Nb)_2Fe$ ternary compound
Cr3Si_A15	Zr_3Sn, Nb_3Sn based solution phase, dissolving other elements
M5SI3_D88	η phase, Zr_5Sn_4 based Zr-rich solution phase, dissolving other elements
MZR3_E1A	$FeZr_3$ compound that forms in Zr-Fe based alloys
Fluorite	γ ZrO_2 phase, high temperature zirconia oxide phase, dissolving other elements
ZRO2_MONO	β ZrO_2 phase, intermediate temperature zirconia oxide phase
ZRO2_TETR	α ZrO_2 phase, low temperature zirconia oxide phase

TCZR1 Models for the Included Phases

Name	*Prototype*	*Pearson*	*Spacegroup*	*Sublattice*	*Notes*
BCC_A2	W	cI2	Im-3m	(Cr, Fe, Nb, Ni, Sn, Va, Zr)1(H, O, Va)3	
BCT_A5	Sn	tI4	I4_1/amd	(Sn)	
C14_LAVES	MgZn2	hP12	P6_3/mmc	(Cr, Fe, Nb, Ni, Sn, Zr)1 (Cr, Fe, Nb,Ni, Sn, Zr)2	>Cr2Zr_ht, Fe2Nb,
C15_LAVES	MgCu2	cF24	Fd-3m	(Cr, Fe, Nb, Ni, Sn, Zr)1 (Cr, Fe, Nb, Ni, Sn, Zr)2	> Cr2Nb, Cr2Zr, Fe2Zr
C16_THETA	Al2Cu	tI12	I4/mcm	(Cr, Fe, Ni)1(Nb, Zr)2	>FeZr2, NiZr2
C36_LAVES	MgNi2	hP24	P6_3/mmc	(Cr, Fe, Nb, Ni, Sn, Zr)1 (Cr, Fe, Nb, Ni, Sn, Zr)2	>(Fe,Nb,Sn)2Zr
CORUNDUM	Al2O3	hR10	R-3c	(Cr+2, Cr+3, Fe+2, Fe+3, Va)2(Cr+3, Fe+3, Ni+2, Va)1 (O-2)3	>Cr2O3
CR3SI_A15	Cr3Si	cP8	Pm-3n	(Cr, Fe, Nb, Ni, Sn, Zr)3 (Cr, Nb, Ni, Sn, Zr)1(Va)3	>Nb3Sn, Zr3Sn
CRNI2_OP6	MoPt2	oI6	Immm	(Cr)1(Ni)2	
DELTA_TIH2	CaF2	cF12	Fm-3m	(Nb, Zr)1(H, Va)2	>NbH2
DIS_MU	Fe7W6	hR13	R-3m	(Cr, Fe, Nb, Ni)	
DIS_SIG	CrFe	tP30	P4_2/mnm	(Cr, Fe, Nb, Ni)	
EPS_ZRH2	ThH2	tI6	I4/mmm	(Zr)1(H)2	
FCC_A1	Cu	cF4	Fm-3m	(Cr, Fe, Nb, Ni, Sn, Zr)1(O, H, Va)1	
FE1SN2	CuAl2	tI12	I4/mcm	(Fe)1(Sn)2	
FE3SN2	Fe3Sn2	hR10	R-3m	(Fe)3(Sn)2	
FE5SN3	Co1.75Ge	hP6	P6_3/mmc	(Fe)5(Sn)3	

Name	Prototype	Pearson	Spacegroup	Sublattice	Notes
FESN	CoSn	hP6	P6/mmm	(Fe)1(Sn)1	
FE23ZR6	Th6Mn23	cF116	Fm-3m	(Fe, Ni, Zr)0.7931(Zr, Fe)0.2069	
FENBZR_TAO1	MgZn2	hP16	P6_3/mmc	(Fe, Nb, Zr)2(Fe, Nb, Zr)1	
FE6SN6ZR	HfFe6Ge6	hP13	P6/mmm	(Fe)0.5(Sn)0.43(Zr)0.07	
FLUORITE_C1	CaF2	cF12	Fm-3m	(Cr+3, Fe+2, Ni+2, Zr, Zr+4)2 (O-2, Va)4	
GAMMA_ZRH	PtS	tP4	P42/mmc	(Zr)1(H)1	
GAS				(Cr, Cr1O1, Cr1O2, Cr1O3, Cr2, Cr2O1, Cr2O2, Cr2O3, Fe, Fe1O1, Fe1O2, Fe2, H, H2, H2O1, H2O2, Nb, Nb1O1, Nb1O2, Ni, Ni1O1, Ni2, O, O1Sn1, O1Zr1, O2, O2Sn1, O2Sn2, O2Zr1, O3, O4Sn4, O6Sn6, Sn, Zr, Zr2	
HALITE	NaCl	cF8	Fm-3m	(Cr+3, Fe+2, Fe+3, Ni+2, Ni+3, Va, Zr+4)1(O-2, Va)1	
HCP_A3	Mg	hP2	P6_3/mmc	(Cr, Fe, Nb, Ni, Sn, Zr)1(H, O, Va)0.5	
HF8NI21	Hf8Ni21	aP29	P-1	(Zr)8 (Fe, Ni)21	>Ni21Zr8
KWON				(Fe)3(Sn)9(Zr)20	>Fe3Sn9Zr20
L10_FCC	CuAu	tP20	P4/mmm	(Ni)0.5(Ni)0.5	
L12_FCC	Cu3Au	cP4	Pm-3m	(Cr, Fe, Ni, Zr)0.75(Cr, Fe, Ni, Zr)0.25	
LIQUID				(Cr, CrO, CrO1.5, Fe, FeO, FeO1.5, H, H2O1, H2O2, Nb, NbO, NbO2, NbO2.5, Ni, NiO, O, Sn, Sn0.5O, Zr, Zr0.5O)	
M5SI3_D88	Mn5Si3	hP16	P6_3/mmc	(Zr)5(Sn)3(Ni, Sn,Va)1	>Zr5Sn4, Zr5Sn3
MU_PHASE	W6Fe7	hR13	R-3m	(Cr, Fe, Nb, Ni)1(Cr, Fe, Nb, Ni)2 (Cr, Fe, Nb, Ni)6(Nb)4	>Fe7Nb6, Ni6Nb7
MZR3_E1A	MgCuAl2	oS16	Cmcm	(Fe, Zr)1(Fe, Zr)3	>FeZr3

Name	Prototype	Pearson	Spacegroup	Sublattice	Notes
NB1O2	NbO2	tI96	I4_1/a	(Nb)1(O)2	
NB2O5	Nb2O5	mP99	P2/m	(Nb)2(O)5	
NBH_BETA	TaH0.5	oS8	C222	(Nb)1(H, Va)1.1	
NBNI8	Pt8Ti	tI18	I4/mmm	(Nb)1(Ni)8	
NBO	NbO	cP6	Pm-3m	(Nb)1(O)1	
NBSN2	Mg2Cu	oF48	Fddd	(Nb)1(Sn)2	
NI3SN2	Ni3Sn2	oP20	Pnma	(Ni, Va)1(Ni, Va)1(Ni, Sn, Zr)1	
NI3SN4	Ni3Sn4	mS14	C2/m	(Ni)0.25(Ni, Sn) 0.25(Sn)0.5	
NI3SN_LT	Mg3Cd	hP8	P6_3/mmc	(Ni, Sn)0.75(Ni, Sn)0.25	
NI2SNZR2	U2SnPt2	tP20	P4_2/mnm	(Ni)2(Sn, Zr)1(Zr)2	
NI2ZRSN	Cu2MnAl	cF16	Fm-3m	(Ni)2(Zr)1(Sn)1	
NISN2ZR6	K2UF6	hP9	P-62m	(Ni)1(Sn, Zr)2(Zr)6	
NISNZR	MgAgAs	cF12	F-43m	(Ni)1(Sn)1(Zr)1	
NI3TA_D0A	Cu3Ti	oP8	Pmmn	(Cr, Fe, Nb, Ni)3(Fe, Nb, Ni)1	>Ni3Nb
NI3ZR	Mg3Cd	hP8	P6_3/mmc	(Ni)3(Zr)1	
NI5ZR	Be5Au	cF24	F-43m	(Fe, Ni, Sn, Zr)5(Zr,Va)1	
NI7ZR2	Ni7Zr2	mS36	C2/m	(Cr, Fe, Ni)7(Zr)2	
NI10ZR7	Ni10Zr7	oS68	Cmce	(Ni)10(Zr)7	
NI11ZR9	Ni11Zr9	tI40	I4/m	(Ni)11(Zr)9	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Sublattice*	*Notes*
NIZR	CrB	oC8	Cmcm	(Ni)1(Zr)1	
N_PHASE	Zr3FE4Sn4	oP44	Pnma	(Fe)16(Sn)16(Zr)12	>Zr3Fe4Sn4
ORD_SIG	Cr0.49Fe0.51	tP30	P4_2/mnm	(Cr, Fe, Nb, Ni)10(Cr, Fe, Nb, Ni)4(Cr, Fe, Nb, Ni)16	
RUTILE_TIO2	TiO2	tP6	P4_2/mnm	(Sn+4, Zr+4)1(O-2, Va-2)2	
SN3O4	Sn3O4	mP14	P2_1/c	(Sn)3(O)4	
SNO	PbO	tP4	P4/nmm	(Sn)1(O)1	
SPINEL	Fe3O4	cF56	Fd-3m	(Cr+2, Cr+3, Fe+2, Fe+3, Ni+2)1(Cr+3, Fe+2, Fe+3, Ni+2, Va,)2 (Cr+2, Fe+2, Va)2 (O-2)4	>Fe3O4
THETA	K2UF6	hP9	P-62m	(Fe)1(Sn)2(Zr)6	>FeSn2Zr6
TISI2_C54	TiSi2	oF24	Fddd	(Nb, Zr)1(Sn)2	>ZrSn2
TI6SN5	Ti6Sn5	oI44	Immm	(Cr, Nb, Zr)6(Sn)5	>Nb6Sn5
XSECONDE				(Fe)8(Sn)20(Zr)18	>Fe4Sn10Zr9
XPRIME				(Fe)9(Sn)20(Zr)22	>Fe9Sn20Zr22
Y				(Fe)18(Sn)9(Zr)5	>Fe19Sn9Zr5
ZRNIO_T				(Ni)1(O, Zr)1(Zr)3	
ZRO2_MONO	ZrO2	tP6	P42/nmc	(Cr+3, Zr+4)2 (O-2, Va)4	
ZRO2_TETR	ZrO2-b	mP12	P121/c1	(Cr+3, Fe+2, Ni+2, Zr+4)2 (O-2, Va)4	

TCZR1 Properties

Model Descriptions

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.

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Examples

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