TCS Ultra-high Temperature Materials Database (TCUHTM1)

Technical Information

Available Starting with Thermo-Calc Version 2022b

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About the TCS Ultra-high Temperature Materials Database (TCUHTM)

The TCS Ultra-high Temperature Materials Database (TCUHTM) is a thermodynamic database for ultra-high temperature materials that can be used for hypersonic aircraft and space vehicles. These are typically non-oxides with melting/decomposition temperatures in excess of 3000 °C. Examples include borides, nitrides, and carbides of Group IV-V metals in the periodic table, such as ZrB_2, HfB_2, ZrC, HfC, TaC, and HfN. SiC was used to improve oxidation resistance. The database can be used to calculate phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria, melting temperatures, and simulating operation processes for a wide range of compositions.

TCS Ultra-high Temperature Materials Database (TCUHTM) is developed to be used with our entire suite of products: Thermo-Calc, the Add-on Modules, and all available SDKs.

The current version of the database is TCUHTM1.

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 area.

The TCS Ultra-high Temperature Materials Database (TCUHTM) enables predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulations, 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 Ultra-high Temperature Materials Database (TCUHTM) 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 Ultra-high Temperature Materials Database (TCUHTM) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, and the phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), and a list of the included elements.
- The *TCS Ultra-high Temperature Materials Database (TCUHTM) 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 Ultra-high Temperature Materials page on our website where you can access an examples collection and the technical information. Also explore further applications of Thermo-Calc 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.

TCUHTM1 Elements, Systems, Phases and Properties

Included Elements

There are 7 elements included in the database.

B	C	Hf	N	Si	Ta	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.

In most cases phases having the same crystal structure had been merged as the same phase.

The database contains:

- 21 assessed binary systems
- 26 assessed ternary systems
- 35 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`.

TCUHTM1 Systems

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TCUHTM1 Assessed Binary Systems

Twenty-one (21) binary systems are assessed.

	C	Hf	N	Si	Ta	Zr
B	X	X	X	X	X	X
C		X	X	X	X	X
Hf			X	X	X	X
N				X	X	X
Si					X	X
Ta						X

TCUHTM1 Assessed Ternary Systems

Twenty-six (26) ternary systems are assessed.

Assessed Ternary Systems							
B-C-Hf	B-C-Si	B-C-Ta	B-C-Zr	B-Hf-N	B-Hf-Si	B-Hf-Zr	B-N-Zr
B-Si-Zr	C-Hf-Si	C-Hf-Ta	C-Hf-Zr	C-N-Si	C-N-Zr	C-Si-Ta	C-Si-Zr
C-Ta-Zr	N-Si-Ta	N-Si-Zr					

Tentatively Assessed Ternary Systems						
B-Hf-Ta	B-N-Ta	B-Ta-Zr	C-Hf-N	C-N-Ta	Hf-N-Si	Hf-N-Ta

TCUHTM1 Phases

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Common Phases for Ultra-high Temperature Materials

TCUHTM1 Models for the Included Phases

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key ultra-high temperature materials.

Name in the Database	*Common Name and Description*
LIQUID	Liquid phase, which covers the melt of ultra-high temperature materials
FCC_B1	Carbide and nitride-based phase, which covers HfC, HfN, TaC, TaN, ZrC, ZrN solution phase compositions.
HCP_A3	Hf, Zr, Ta2C, Ta2N solution phase
BCC_A2	Hf, Ta, Zr solution phase
MB2_C32	It covers HfB2, TaB2, ZrB2
M5Si3_D88	It covers Hf5Si3, Zr5Si3, Hf5Si3B, Hf5Si3C, Zr5Si3C, Zr5Si3N

TCUHTM1 Models for the Included Phases

The table lists all phases and the thermodynamic model used to describe the phase.

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Sublattice*	*Notes*
B12ZR	UB12	cF52	Fm-3m	D2f		(B)12(Zr)1	
B3SI	B13C2	hR15	R-3m	D1g	166	(B)6(Si)2(B, Si)6	
B4C	B4C	hR15	R-3m	D1g	166	(B11C, B12)1(B2, C2B, CB2, Si2)1	
B6SI	B6Si	oP280	Pnnm			(B)210(Si)23(B, Si)48	
BCC_A2	W	cI2	Im-3m	A2	229	(Hf, Si, Ta, Va, Zr)1(B, C, N, Va)3	Hf, Ta, Zr Body-Centered Cubic
BETAR_BORON	B	hR105	R-3m		166	(B)93(B, C, Si)12	
BNSI	B	hR12	R-3m		166	(B)61(Si)1(B, Si)8	BnSi
BN_B4	ZnS, B4	hP4	P6_3/mmc	Bk	194	(B)1(N)1	Wurtzite
C16_THETA	Al2Cu	tI12	I4/mcm	C16	140	(Hf, Ta, Zr)2(Si)1	Hf2Si, Zr2Si
CRSI2_C40	CrSi2	hP9	P6_222	C40	180	(Hf, Si, Ta)1(Si)2	TaSi2, ZrSi2
D5A_M3B2	Si2U3	tP10	P4/mbm	D5a	127	(Hf, Ta)3(B)2	Ta3B2
DIAMOND_A4	C	cF8	Fd-3m	A4	227	(B, C, Si)1	Si
FCC_B1	NaCl	cF8	Fm-3m	B1	225	(Hf, Ta, Va, Zr)1 (B, C, N)1	HfC, HfN, TaC, TaN, ZrC, ZrN solution phase
GAS						(B, B1C1, B1C2, B1N1, B2, B2C1, C, C1N1, C1N2_CNN, C1N2_NCN, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2N1_CCN, C2N1_CNC, C2N2, C2SI1, C2SI2, C2SI3, C3, C3N1, C4, C4N1, C4N2, C5, C5N1, C60, C6N1, C6N2, C9N1, HF, N, N1SI1, N1SI2, N1ZR1, N2, N3, SI, SI2, SI3, Ta, Zr ZR2)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
GRAPHITE	C	hP4	P6_3/mmc	A9	194	(B, C)1	
HCP_A3	Mg	hP2	P6_3/mmc	A3	194	(Cr, Fe, Nb, Ni, Sn, Zr)1(H, O, Va)0.5	Hf, Zr, Ta2C, Ta2N solution phase
HF3N2	TiS	hR18	R-3m		166	(Hf)0.64(N)0.36	
NF4N3	Sc2Te3	hR8	R-3m		166	(Hf)0.61(N)0.39	
LIQUID						(B, C, Hf, N, Si, Ta, Zr)	
M2B_TETR	Al2Cu	tI12	I4/mcm	C16	140	(Ta)2(B)1	Ta2B
M3SI1	Ti3P	tP32	P4_2/n		86	(Hf, Ta, Zr)3(Si)1	Ta3Si, Zr3Si
M3SI2_D5A	Si2U3	tP10	P4/mbm	D5A	127	(Hf, Zr)2(Si)2	Hf3Si2, Zr3Si2
M5SI3_D88	Mn5Si3	hP16	P6_3/mmc	D88	193	(Hf, Zr)3(Si)3(B, C, N, Va)1	Hf5Si3, Zr5Si3, Hf5Si3B, Hf5Si3C, Zr5Si3C, Zr5Si3N
MB2_C32	AlB2	hP3	P6/mmm	C32	191	(B)2(B, Hf, Ta, Zr)1	HfB2, TaB2, ZrB2
MB_B33	CrB	oS8	Cmcm	B33	63	(Hf, Ta, Zr)1 (B)1	TaB, ZrB
MSI_B27	FeB	oP8	Pnma	B27	62	(Hf, Zr)1(Si)1	HfSi, ZrSi
SI3N4	Si3N4	hP28	P31c		159	(Si)3(N)4	
SIC	ZnS	cF8	F-43m	B3	216	(Si)1(B, C)1	
TA5SI3C						(Ta)5(Si)3(C, N, Va)1	Ta5Si3C, Ta5Si3N
TA5SI3_D8L	Cr5B3	tI32	I4/mcm	D8l	140	(Hf, Ta)5(Si)3	Low temperature Ta5Si3
TA5SI3_HT	W5Si3	tI32	I4/mcm	D8m	140	(Ta)5(Si)3	High temperature Ta5Si3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Sublattice*	*Notes*
TI3B4	Ta3B4	oI14	Immm	D7b	71	(B)4(Hf, Ta)3	Ta3B4
TIB_B27	FeB	oP8	Pnma	B27	62	(B)1 (Hf, Ta, Zr)1	HfB
ZR5SI4	Cr5B3	tI32	I4/mcm	D8l	140	(Hf, Zr)5(Si)4	Zr5Si4, Hf5Si4
ZRSI2_C49	ZrSi2	oS12	Cmcm	C49	63	(Hf, Zr)1(Si)2	ZrSi2, HfSi2