TCFE7: TCS Steel and Fe-alloys Database

Thermo-Calc Software is pleased to announce the release of TCFE7, a thermodynamic database for different kinds of steels and Fe-based alloys (stainless steels, high-speed steels, tool steels, HSLA steels, cast iron, corrosion-resistant high strength steels and more) for use with the Thermo-Calc, DICTRA and TC-PRISMA software packages. In order to increase the predictive capability of the database, several significant re-assessments have been performed by Thermo-Calc Software AB which are incorporated in the new release. The elements Ta and Zr and relevant phases associated with these elements have been added. Three more B containing phases and two more Mn nitride phases have been also implemented into the new TCFE7 database. All oxide phases for the Fe-Al-Ca-Cr-Mg-Mn-Ni-Si-O system have been updated or added, which includes the addition of many new oxide phases.Within the latter system all lower-order sub-systems have been evaluated.

In version 4 (TCFE4), all necessary volume data (including molar volume and thermal expansion) for various alloy phases were incorporated; such volume data has been updated for all phases in this new release. However, the molar volume data incorporated has no pressure dependence.

Some of the major improvements to the TCFE7 database include improved/added thermodynamic descriptions for the following binary, ternary and quaternary systems (with many sub-systems also re-assessed):

Al-Ta	B-Ta	C-Ta	Co-Ta
Cr-Ta	Cu-Ta	Fe-Ta	Mn-Ta
Mo-Ta	N-Ta	Nb-Ta	Ni-Ta
Si-Ta	Ta-Ti	Ta-V	Ta-W
Ta-Zr	Al-Zr	B-Zr	C-Zr
Co-Zr	Cr-Zr	Cu-Zr	Fe-Zr
Mg-Zr	Mn-Zr	Mo-Zr	N-Zr
Nb-Zr	Ni-Zr	O-Zr	S-Zr
Si-Zr	Ti-Zr	V-Zr	W-Zr
Al-N-Ta	C-Cr-Ta	C-Fe-Ta	C-Mo-Ta
C-Ta-W	C-Ta-Zr	C-Ta-Ti	C-Ta-V
N-Nb-Ta	N-Ta-Ti	Al-Co-Zr	Al-Cr-Zr
C-Co-Zr	C-Cr-Zr	C-Mo-Zr	C-Ni-Zr
C-Ti-Zr	C-V-Zr	C-W-Zr	Co-Ti-Zr
Co-W-Zr	Cr-Ni-Zr	Cr-W-Zr	Fe-Nb-Zr
Ni-W-Zr	Ti-W-Zr	C-Fe-Zr	Fe-N-Zr
Zr-C-N	Ti-Zr-W-C	Co-W-C-Ta	B-Cr

B-Fe	B-Mn	B-Mo	B-Nb
B-Ni	B-Ta	B-Ti	B-V
B-W	B-Cr-Fe	Fe-Nb	Fe-Nb-C
Fe-Cr-W	Fe-Mn-N	Al-Cr-O	Al-Fe-O
Al-Mn-O	Al-Ni-O	Ca-Cr-O	Ca-Mn-O
Ca-Ni-O	Cr-Mg-O	Cr-Si-O	Fe-Mg-O
Mg-Mn-O	Mg-Ni-O	Mn-Si-O	Ni-Si-O
Al-Ca-Mg-O	Al-Ca-Si-O	Ca-Mg-Si-O	Ca-Fe-Si-O
Fe-Cr-Mn-O	Fe-Cr-Ni-O	Cr-Mn-Ni-O	Fe-Mg-Si-O

Compared with the previous version TCFE6 v6.2 the new phases in the TCFE7 database are as listed below:

BM	M3B2	MB_B33
MN6N4	MN6N5	TAN_EPS
S2ZR1	ZR2S3	ZRO2_MONO
ZRO2_TETR	RHODONITE (formerly MNO_SIO2)	OLIVINE (Ca, Fe, Mg, Mn, Ni, Si, O)
MN2O3	NI6MNO8	NIMNO3
CORUNDUM	HALITE	ALPHA_SPINEL
SPINEL	CAMNO3	CAMN2O4
CA1CR2O4_A	CA1CR2O4_B	C1A1
AF	CF	C1A2
CF2	C1A6	C2F
C3A1	CWF	CW3F
C4WF4	C4WF8	C3A2M1
C1A8M2	C2A14M2	FESO4
FLUORITE_C1	G_PHASE	CORDIERITE
SAPPHIRINE	CA2SIO4_ALPHA	CA2SIO4_ALPHA_PRIME
LARNITE	LOWCLINO_PYROXEN	CLINO_PYROXENE

ORTHO_PYROXENE	PROTO_PYROXENE	WOLLASTONITE
PSEUDO_WOLLASTONITE	ANDALUSITE	SILLIMANITE
MULLITE	KYANITE	HATRURITE
MELILITE	ANORTHITE	MERWINITE

In addition to this, many new elements are modelled to dissolve in more phases such as Boron containing phases, LAVES_PHASE, nitrides, oxides etc. A comprehensive list of how the different phases are modelled (number of sub-lattices and atomic ratio), and which elements/constituents they contain, can be found in the extended information flyer for the TCFE7 database. In that document validation data for various types of alloys are presented as well.

The LIQUID, MU_PHASE and SIGMA phases have been improved due to the modifications for the MU_PHASE in the Fe-Nb system, SIGMA phase in the Fe-Cr-W system, LIQUID in the Fe-Nb-C and C-Fe-O systems.

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