Thermo-Calc 2017a: Major Updates to the TCFE9 Steel and Fe-alloys Database

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The TCS Steel and Fe-alloys Database, referred to as TCFE9, is a thermodynamic database for different kinds of steels and Fe-based alloys, such as stainless steels, high-speed steels, tool steels, high-strength low alloy (HSLA) steels, cast irons, corrosion-resistant high strength steels, low-density steels, and also cemented carbides.

The database is developed and validated for simulation of the solidification process, the relative stability of matrix phases (austenite and ferrite), precipitation of secondary phases such as sulfides, borides, oxides, phosphides, carbides, nitrides, carbonitrides, and also intermetallic phases such as the sigma and laves phases.

The TCFE9 database is significantly improved compared to the previous TCFE8 version, with 32 new binary and 35 new ternary systems added to the database. In addition, more than 50 binary and 39 ternary, and many quaternary, systems are either completely updated or partially modified to improve the robustness and predictability of the database. The included systems are listed in Table 2, Table 3, and Table 4.

The major improvements to the TCFE9 database are as follows:

A new element: Cerium (Ce)

Cerium (Ce) is added with 19 Ce-X binary systems (X=Al, B, C, Ca, Co, Cr, Cu, Fe, Mg, Mn, Mo, Ni, O, S, Si, V, Y, Zn, Zr). Two examples are shown in Figure 1.

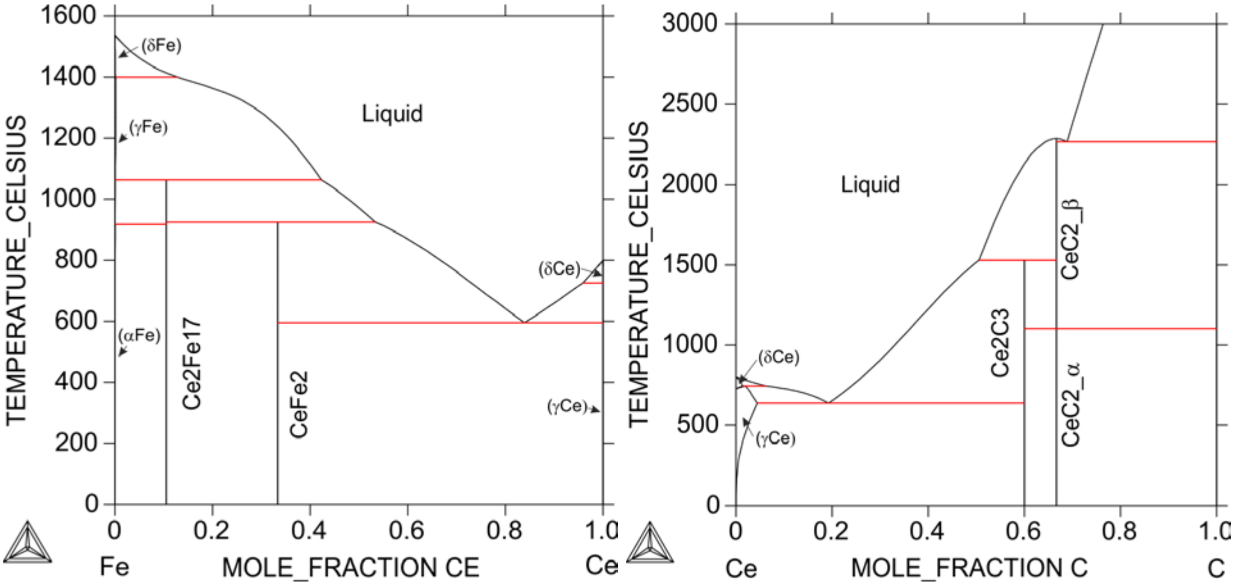

Figure 1. Phase diagram of a) Ce-Fe [2005, Su] and b) C-Ce [2011, Peng] systems.

Sulphurous systems

The formation of sulfides in steels can be detrimental or beneficial. In either case it is important to understand and control the formation of sulfides. In the TCFE9 database the thermodynamics of Ca-Fe-Mn-Mg-S and its lower order systems are updated after the work by Dilner [2016] (Figure 2). The Cr solubility in MnS is estimated based on the experimental data. Cu-sulfides are also added for some applications such as electrical steels.

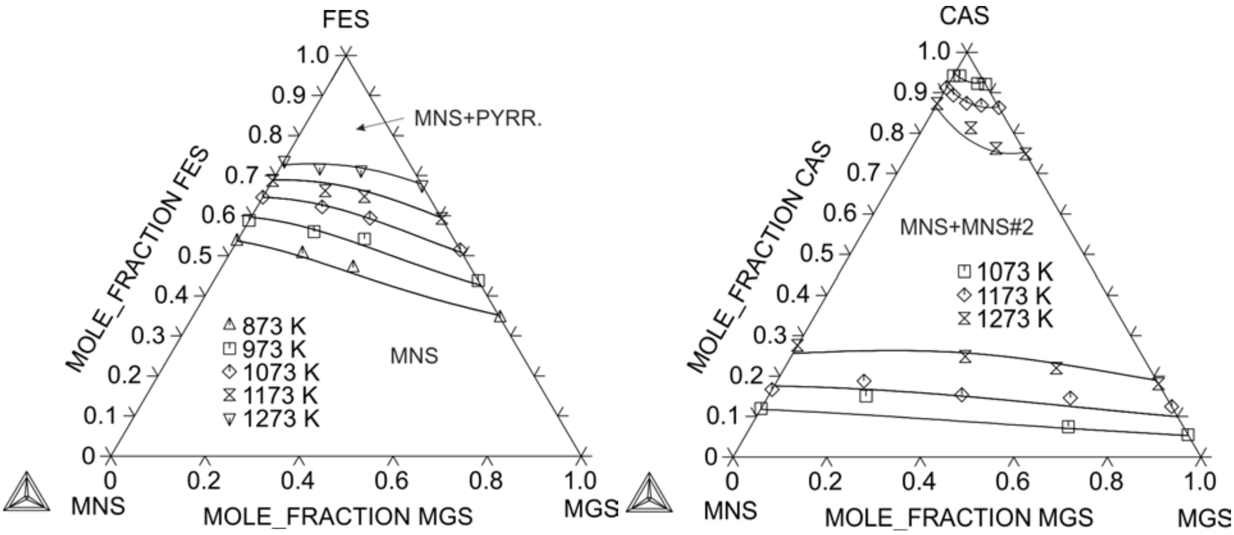

Figure 2. a) The solubility lines in the FeS-MnS-MgS system in the temperature interval 873-1273 K. b) The CaS-MgS-MnS isothermal sections plotted at 1073-1273 K together with experimental information as cited in [2016, Dilner].

Phosphorous systems

Recently a series of new experimental data and thermodynamic assessments regarding the phosphorus containing systems became available [2014a, 2014b and 2015, Miettinen]. Thereafter, several phosphorus containing ternary iron-based systems, Fe-X-P (X=Al, Cr, Mn, Mo, Nb, Ni, Ti, Si) are included in the TCFE9 database.

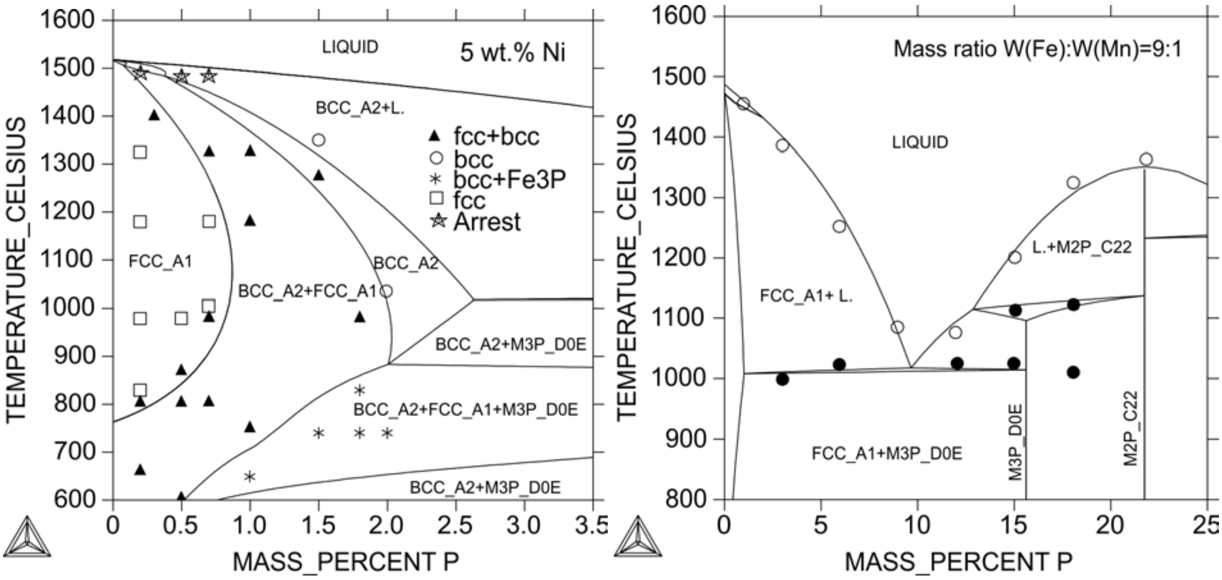

Figure 3. a) The vertical section of the Fe-Ni-P system at 5 wt.% Ni, together with experimental data as cited in [2015, Miettinen]. b) Calculated vertical section of the Fe-Mn-P system at mass ratio W(Fe):W(Mn)=9:1, together with experimental data as cited in [2014b, Miettinen].

Boron-containing systems

Thermodynamic description of many boron containing systems are revised including iron containing ternary systems, Fe-X-B (X=C, Cr, Co, Mo, Mn, Nb, Ni, Si, Ti, V, W, Zr), and also some other ternary systems such as B-Cr-Mo, B-Cr-Ni, B-Ni-Si and the quaternary B-Cr-Fe-Mo system.

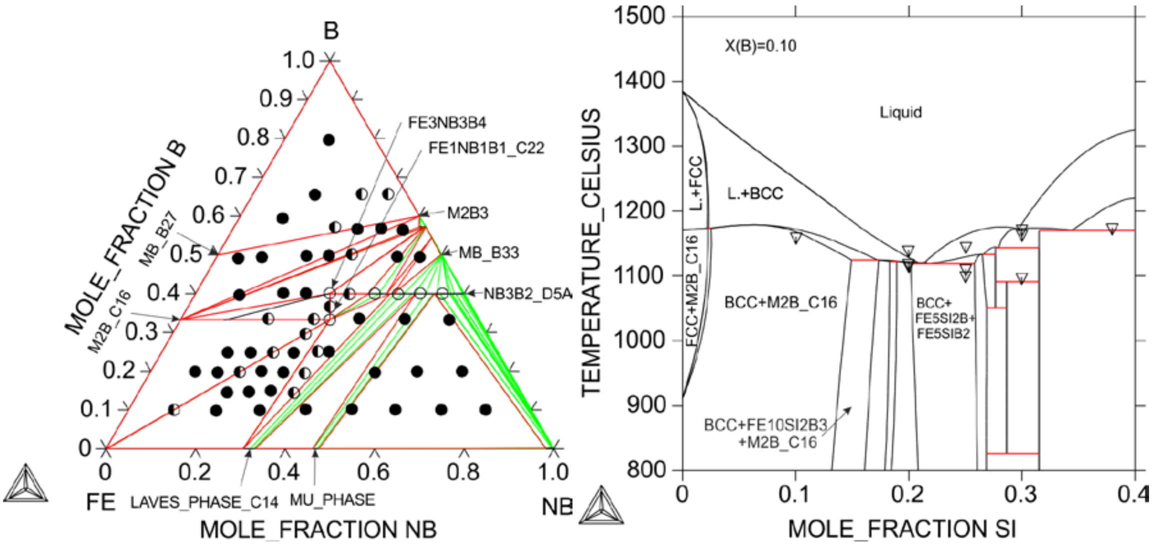

Figure 4. a) A calculated isothermal section diagram of the Fe–Nb–B system at 1073 K, compared with the experimental phase fields [2008, Yoshitomi].b) Calculated Fe-Si-B isopleth at X(B)=0.10 with DSC data [2013, Poletti].

Laves phase

In the TCFE9 database, vanadium (V) is added in the Laves phase and the solubility of many elements are revised. The Laves phase is modified in Fe-Nb, Cu-Mo, Cu-Nb, Cu-W, Mo-Si, Nb-Si, Cu-Fe-Mo, Cr-Fe-Mo, Cr-Si-Nb, Fe-Mn-Mo, and Fe-Mo-Si systems. This description shows satisfying accuracy of the predictions compared to experimental information [2008, Zhang; 2000, Wang].

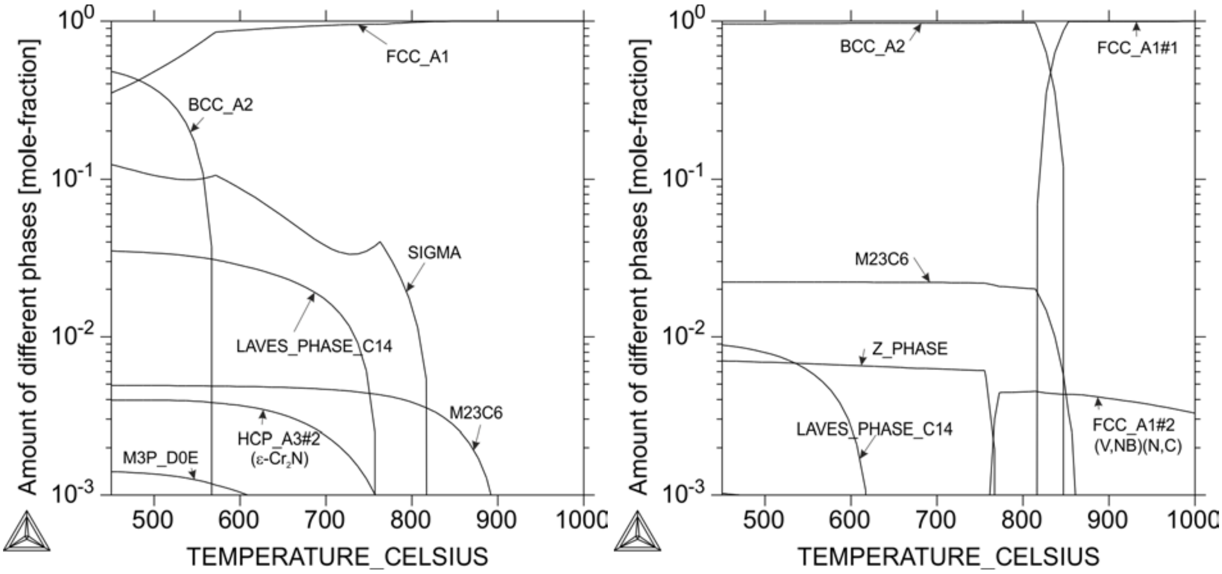

Figure 5. Amount of different phases as a function of temperature in two commercial steels a) 316L [2004, Sahlaoui] b) P91 [2010, Panait].

Copper-containing systems

The thermodynamic properties of Cu contacting systems is improved by adding several new descriptions including Ca-Cu, Cu-Nb, Cu-W, Al-Cu-Fe, Al-Cu-Mn, Al-Cu-Ni, Cr-Cu-Mo, Cr-Cu-W, Cu-Fe-Mn (Figure 6a), Cu-Fe-Mo (Figure 6b) and Cu-Mn-Ni systems.

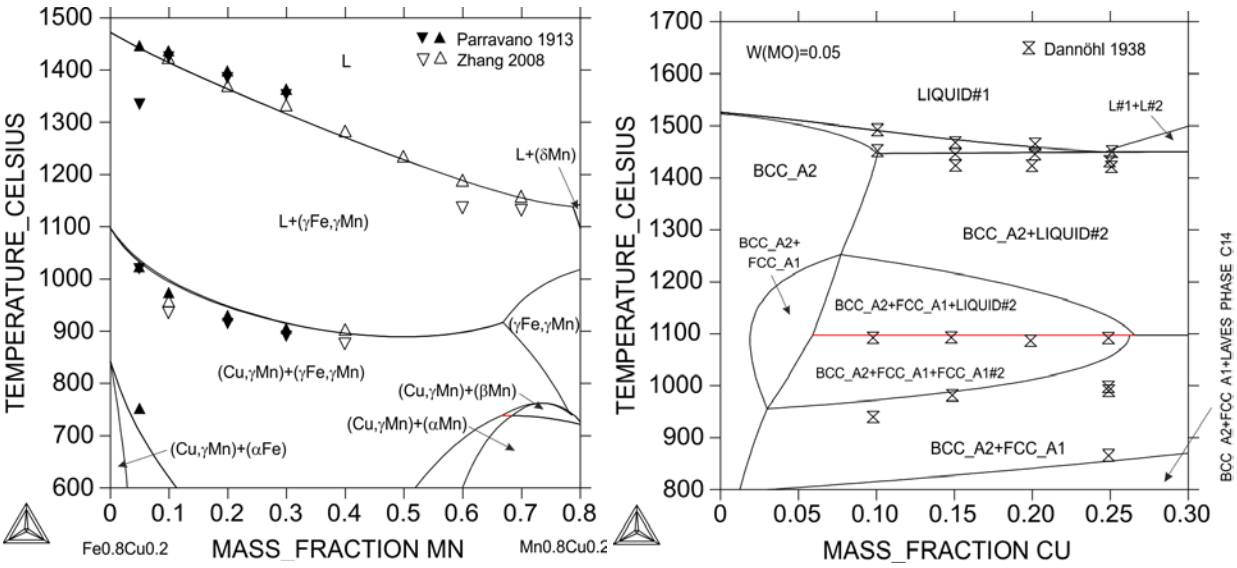

Figure 6. a) Calculated vertical sections of the a) Cu-Fe-Mn system at 20 wt.% Cu [2008, Zhang]. b) Cu-Fe-Mo system at 5 wt.% Mo along with the experimental data [2000, Wang].

Nb and V-containing systems

Niobium (Nb) and vanadium (V) are common alloying elements in different types of steels with high affinity to form carbides and nitrides. In the TCFE9 database several Nb and V systems are either newly added (such as Mn-Nb and Fe-Mn-Nb (Figure 7a) systems) or updated (including C-Nb, Fe-Nb, Fe-V, Nb-V, C-Cr-Nb, and Fe-Nb-V (Figure 7b)).

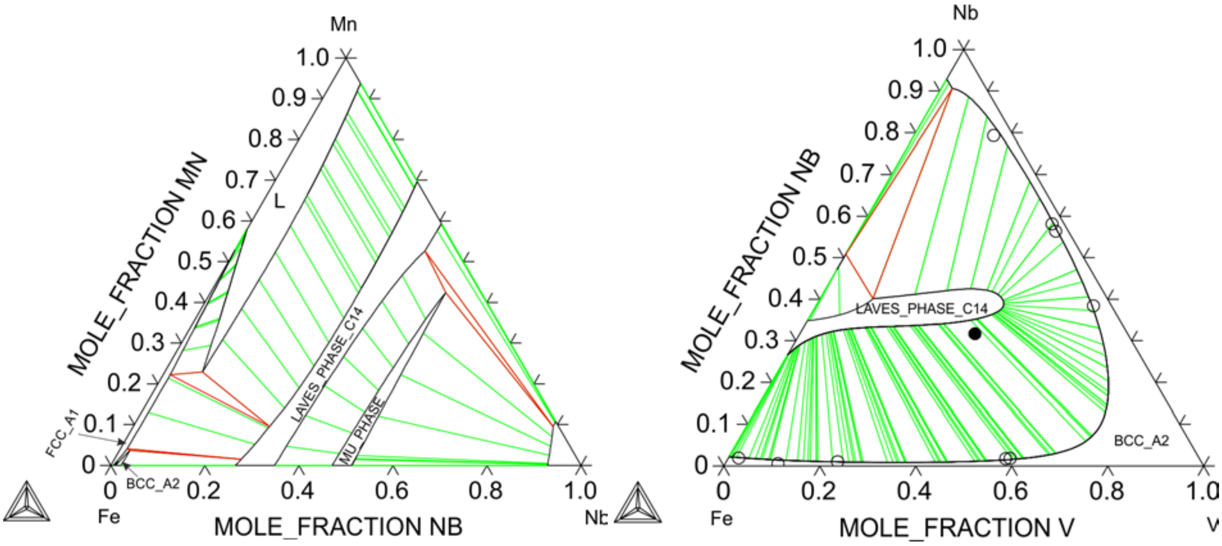

Figure 7. Isothermal sections of a) Fe-Mn-Nb [2013a, Khvan] and b) Fe-Nb-V [2013b, Khvan] systems at 1573 K.

Peritectic reaction and continuous casting

High temperature equilibria, and specifically the peritectic reaction, is of significant importance in continuous casting practice. The TCFE9 database is improved by using data from recent thermodynamic assessments [2017, Zheng] and systematic DSC measurements in C-Fe-Mn-Si and Al-C-Fe-Mn-Si systems.

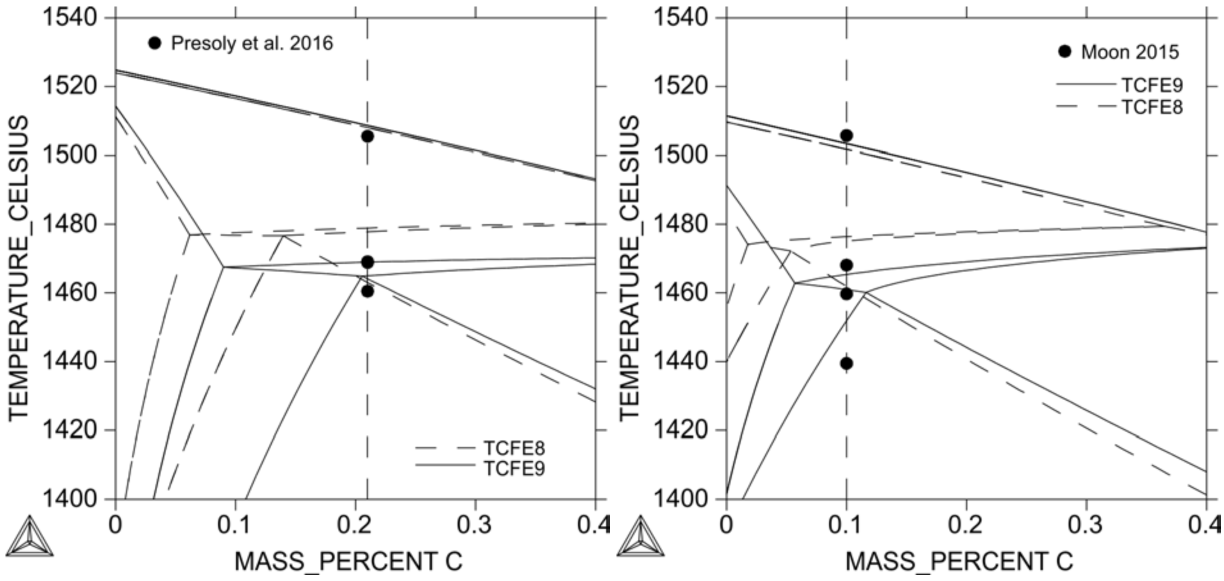

Figure 8. a) Calculated isoplethal section of a) Fe-2.12Mn-0.77Al-0.54Si-xC b) Fe-2.75Mn-1.11Si-0.097Al-0.014Ti-0.02Nb-xC

Low-density steels

Reducing the weight of engineering structures saves both material and energy, and also leads to greater fuel efficiency and reduces emissions in automobiles.

The Al-C-Cr-Fe-Mn-Ni systems is the core of low density steels and allows studies to replace costly Ni and Cr in stainless steels by cheaper Mn and Al. In the TCFE9 database the Al-C-Cr-Fe-Mn-Ni and its subsystems are updated with the latest assessments and experimental info. The Kappa phase is described with a regular CEF model and extended with Mn. Manganese phases CBCC_A12 and CUB_A13 are also added.

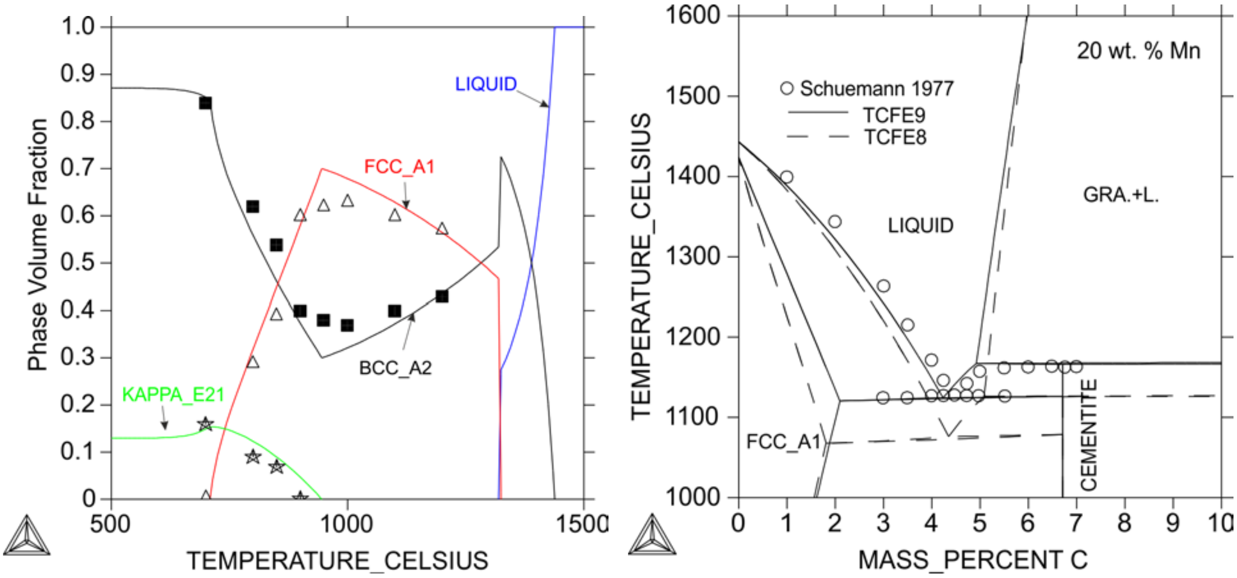

Figure 9. a) The mole fraction change of each phase with the temperature for Fe-10Mn-10Al-0.7C low-density steel [2016, Zhao]. b) The calculated vertical section of C-Fe-Mn involving the liquid phase at 20 wt.% Mn [2011, Djurovic].

Ordered phases

The ordered phases B2_BCC and L12_FCC are described based on the order/disorder partitioning model as described by Lukas et al. [2007]. In the TCFE9 database the ordered phases B2_BCC and L12_FCC are extended to contain the same elements as the corresponding disordered parts (BCC_A2 and FCC_A1). However, the ordering parameters are only assessed in the systems where the ordering is of significant importance. These phases are rejected by default and can be restored manually if required.

In the TCFE9 database the B2_BCC phase is revised in Al-Co, Al-Cr, Al-Ni, Co-Fe, Cr-Ni and Al-Cr-Ni, Al-Fe-Mn (Figure 10a), Al-Fe-Ni (Figure 10b), Al-Mn-Ni, Al-Co-Ni, and Co-Cr-Ni systems.

In addition to the B2_BCC phase, the L12_FCC phase is revised in Al-Cu, Cu-Fe, Cu-Ni, Cr-Ni, Cr-Fe, and Al-Cr-Ni, Al-Fe-Ni (Figure 10b), Al-Mn-Ni, Cr-Fe-Ni, Al-Co-Ni, and Co-Cr-Ni systems.

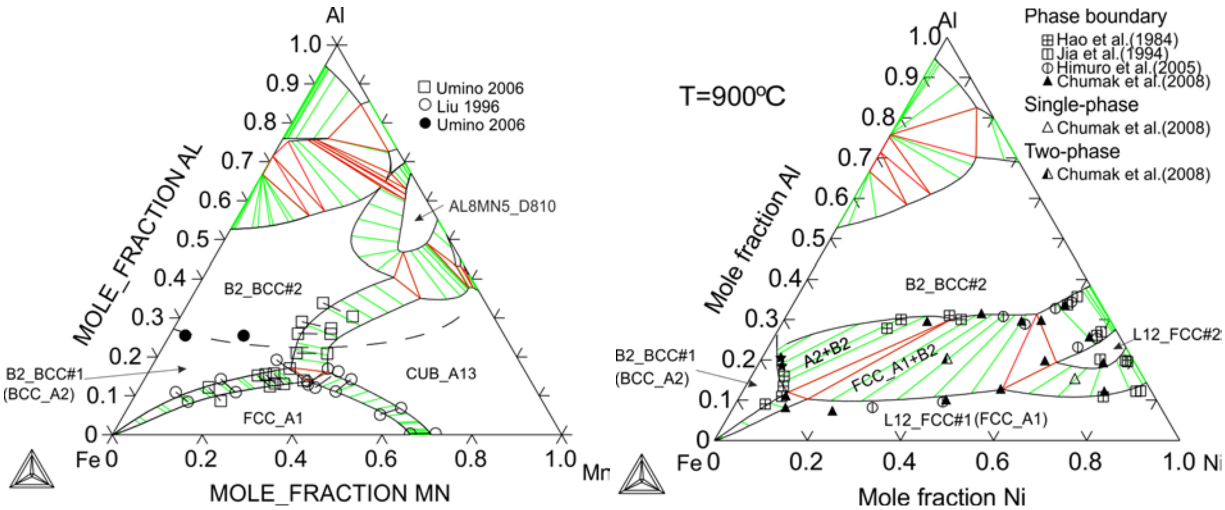

Figure 10. Isothermal section of a) Al-Fe-Mn and b) Al-Fe-Ni at 900 °C compared with the experimental data.

Recently Kim et al. [2015] showed that a B2-type brittle but hard intermetallic compound can be effectively used as a strengthening second phase in high-aluminum low-density steel. Table 1 shows the result of a calculation with the TCFE9 database compared with the experimental observations of Kim et al. [2015].

Table 1. Partitioning of alloying elements between B2 precipitate and austenite matrix in during annealing of cold rolled Fe-10Al-15Mn-0.8C-5Ni (at.%). Calculation with the TCFE9 database vs. experimental data [2015, Kim].

	FCC_A1 composition (at.%)		**B2_BCC composition (at.%)**	
Element	**Calculated**	**Experiment [19]**	**Calculated**	**Experiment [19]**
Fe	65.6	68	53.7	57
Al	15.1	13	25.5	22.6
Mn	16.8	16.6	10.2	9.4
Ni	1.9	2.4	10.1	11.0

Epsilon martensite

The TCFE9 database has been successfully used for thermodynamically-based prediction of the lath and plate martensite start temperature [2012, Stormvinter]. The Ms temperature prediction depends on the available driving force which should be equal to the barrier for Martensite formation. In the TCFE9 database particular attention is paid to the epsilon (ε) martensite transformation, and the thermodynamic descriptions of the Fe-C and Fe-Mn-C systems are modified to give a reasonable driving force for the γ→ε diffusionless transformation. As a result, the database can be used with a user defined model, similar to Stormvinter [2012], to predict the (ε) martensite Ms temperature (Figure 11).

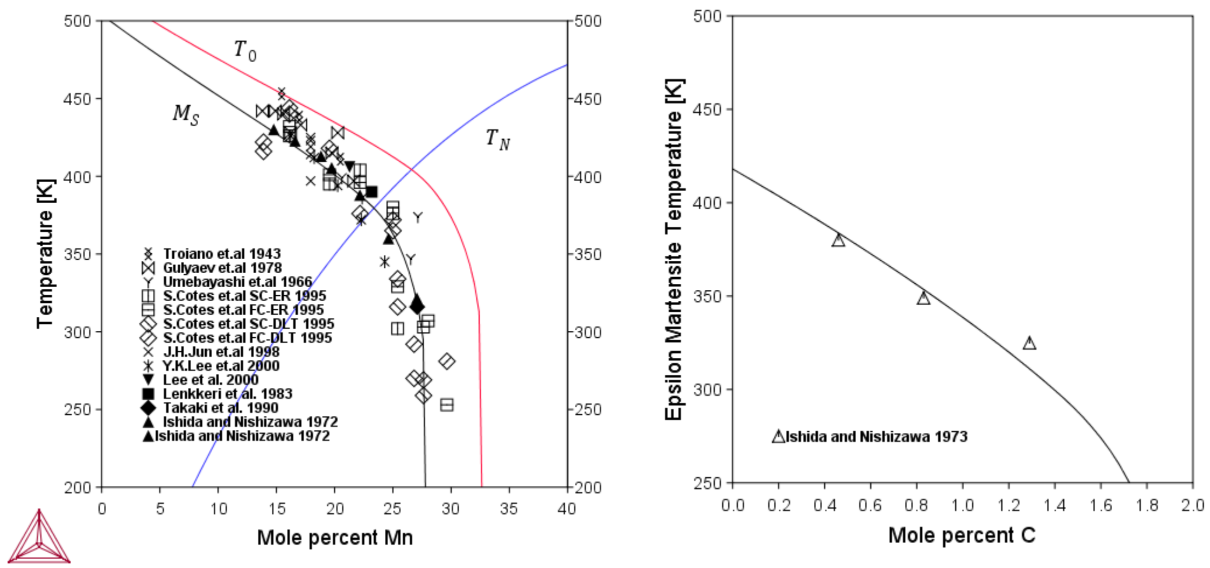

Figure 11. Epsilon martensite start temperature a) Fe-Mn, b) Fe-17at.% Mn-xC

Assessed binary systems

Table 2. The 255 binary systems including 32 newly added (■) and 50 updated (■) in TCFE9 database.

	Al	B	C	Ca	Ce	Co	Cr	Cu	Fe	Mg	Mn	Mo	N	Nb	Ni	O	P	S	Si	Ta	Ti	V	W	Y	Zn	Zr
Al	Al																									
B		B																								
C			C																							
Ca				Ca																						
Ce					Ce																					
Co						Co																				
Cr							Cr																			
Cu								Cu																		
Fe									Fe																	
Mg										Mg																
Mn											Mn															
Mo												Mo														
N													N													
Nb														Nb												
Ni															Ni											
O																O										
P																	P									
S																		S								
Si																			Si							
Ta																				Ta						
Ti																					Ti					
V																						V				
W																							W			
Y																								Y		
Zn																									Zn	
Zr																										Zr

Assessed ternary systems

Table 3. The 255 ternary systems including 35 newly added (■) and 39 updated (■) in the TCFE9 database.

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

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

Assessed quaternary systems

Table 4. The 77 quaternary systems including 2 newly added (■) and 9 updated (■) in the TCFE9 database.

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

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