

TCFE: Major Updates from TCFE9 to TCFE10



There is also the complete [TCFE history available on the website](#).

The TCFE10 database, released with Thermo-Calc version 2020a, is significantly improved compared to TCFE9:

- 53 new binary and 13 new ternary systems are included.
- More than 15 binary and 14 ternary systems, and many quaternary, are either completely updated or partially modified to improve the database's robustness and predictability.

The major improvements to the TCFE10 database are as follows.

Ruthenium (Ru) Systems

Ruthenium (Ru) is added to the database with 19 Ru-X binary systems (X=Al, B, C, Ca, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, S, Si, Ta, Ti, V, Zn). In addition, the Cr-Fe-Ru is assessed at the Fe corner.

Better Predictive Capacity for Nitrogen Alloyed Duplex Stainless Steels

The systems relevant for nitrogen alloyed duplex stainless steels were systematically reviewed and revised as necessary.

The database predictivity is improved in these critical areas:

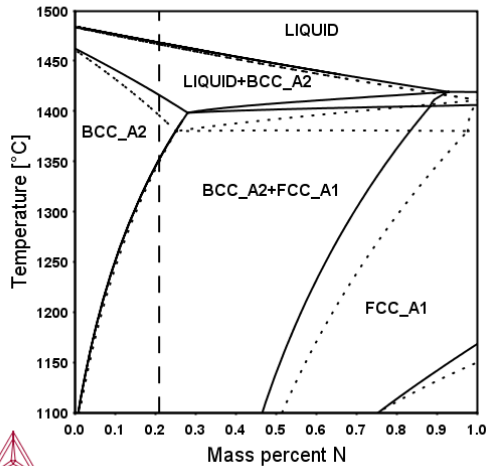
- Equilibria at liquidus - solidus
- Equilibria of matrix phases ($\alpha+\gamma$) at high temperature
- Equilibria of secondary phases at intermediate temperature

The duplex steels are designed to solidify in the single-phase ferritic mode with formation of austenite by precipitation in the solid state [1992 Nilsson, 2017 Petterson]. The high-temperature phase equilibria calculations with TCFE10 show an interval below solidus where the material is fully ferritic ([Figure 1](#)).

2019.11.07.13.30.54

TCFE10: C, CR, CU, FE, MN, MO, N, NI, SI

W(C)=2.1E-4, W(SI)=6.6E-3, W(MN)=4.86E-2, W(CR)=0.2127, W(NI)=1.64E-2, W(MO)=2E-3, W(CU)=2.4E-3, P=1E5, N=1



2019.11.07.13.34.42

TCFE10: C, CR, CU, FE, MN, MO, N, NI, SI

W(C)=1.2E-4, W(SI)=3E-3, W(MN)=8.3E-3, W(CR)=0.2484, W(NI)=6.9E-2, W(MO)=3.8E-2, W(CU)=1.8E-3, P=1E5, N=1

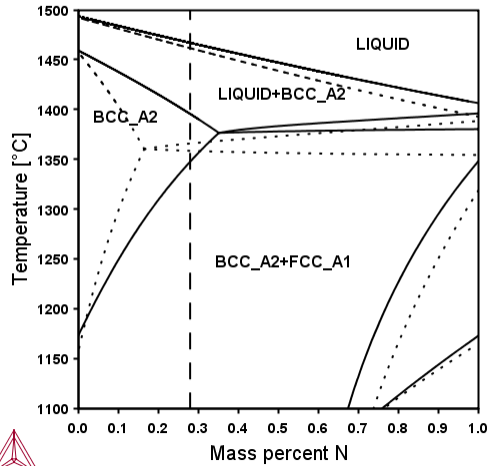


Figure 1: Calculated isopleth sections for 2101 grade (left) and 2507 grade (right) with nitrogen contents up to 1 wt. % using the TCFE10 database (solid lines) compared with TCFE9 (dotted line). The nitrogen content of the alloy is indicated by the dashed lines.

The new assessment of the Cr-Fe-N system agrees well with the experimental observations of nitride formation at nitrogen activity of 0.5 and 1 as shown in Figure 2 (left). The effect of other alloying elements on the FCC/HCP boundary is shown in Figure 2 (right).

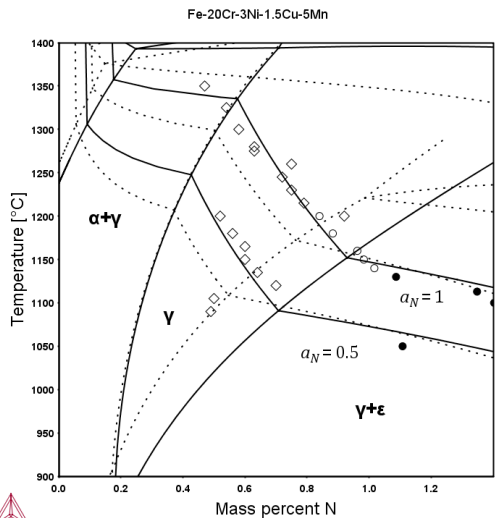
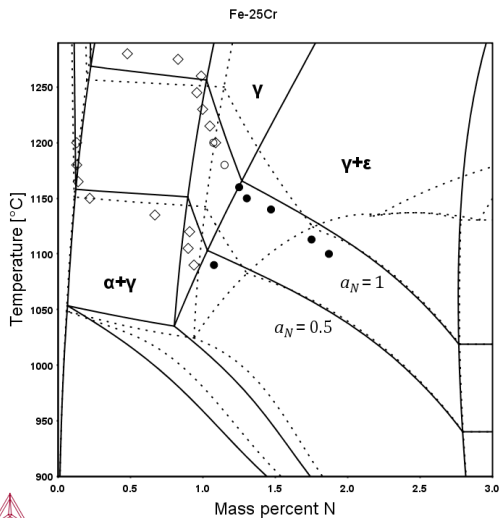


Figure 2: Isopleth for the Fe-25Cr and Fe-20Cr-5Mn-3Ni-1.5Cu-N system calculated with TCFE10 (solid lines) showing the phase regions of main interest and the isoactivity line $a_N = 1$ and the iso-activity line for $a_N = 0.5$. Using the TCFE10 database (solid lines) compared with TCFE9 (dotted line). Experiments from FROST project – Internal report.

New Phases and Crystallographic Information for all Phases



The crystal structure information for all included phases in the TCFE10 database is listed in [Included Phases in TCFE10](#). Similar information is also available when working in the Console Mode by using the DATABASE_RETRIEVAL module. You can display the information using the LIST_SYSTEM CONSTITUENTS and after the systems are defined.

TCFE10 database contains 31 new phases among which the so called η -silicide (η -nitride) is named as ETA_M5SiN; and τ 1-silicide ($\text{Fe}_{2.5}\text{Ni}_{1.5}\text{Si}$) and π -silicide ($\text{Cr}_{1.5}\text{Ni}_{2.5}\text{Si}$) are modeled as M4Si1_G3.

The η -silicide has a diamond cubic structure with typical composition $\text{Cr}_3\text{Ni}_2\text{SiN}$. Fe was identified to substitute Ni and Mo to substitute Cr. Therefore, the model used in the database is $\text{Cr,Mo}_3(\text{Fe,Ni})_2\text{Si}_1\text{N}_1$. Experimental information found in the literature together with new experimental information within internal projects were used to assess the thermodynamic description of the η -silicide.

In [Table 1](#) the composition of the alloys studied are shown and in [Table 2](#) a comparison is made between observed and calculated amount of η -silicide.

Table 1. Composition (wt. %) of two of the alloys studied by Petterson (1998).

Alloy	C	Si	Mn	P	S	Cr	Ni	Mo	N
B3	0.014	0.54	1.44	0.009	0.003	19.8	25.0	4.59	0.21
L3	0.014	0.56	5.24	0.012	0.004	20.2	18.5	4.28	0.44

Table 2. Comparison between measured and calculated composition of η -silicide in alloys B3 and L3 at 800 °C (from [1998 Petterson]).

Alloy	at. %	Cr	Ni	Mo	Fe	Si	N
B3	Exp.	30	25.5	12	5	13	14.5
	Calc.	27.7	25.8	15.2	2.8	14.3	14.3
L3	Exp	24	25.0	15.0	4.5	13	18.5
		25.1	24.7	15.2	8.0	(14.3)	(14.3)
	Calc.	28.6	26.3	14.3	2.3	14.3	14.3

Viscosity of the Metallic Liquid

In the TCFE10 database, the viscosity of metallic liquid alloys is modeled as follows:

$$RT \ln \eta = RT \ln \eta_0 + E$$

where η is the dynamic (or shear) viscosity of the liquid and η_0 is the viscosity at finite temperatures, E is the activation energy in J/mole, R is the gas constant and T absolute temperature. The SI unit of viscosity is pascal.second (Pa.s). The viscosity parameters are expanded via Redlich-Kister polynomials. Example: Viscosity of a liquid A-B alloy is:

$$RT \ln \eta_{\text{alloy}} = x_A(E_A + RT \ln \eta_0^A) + x_B(E_B + RT \ln \eta_0^B) + x_A x_B [L_0 + (x_A - x_B) \cdot L_1]$$

The two first terms are the contributions for the end-members, A and B elements and the last term accounts for the excess viscosity. Basically, we optimize the activation energies. L_0 , L_1 and etc. are the parameters that are optimized to fit the viscosity data.

The kinematic viscosity, ν , is the ratio of the dynamic viscosity to the density, ρ , of the alloy:

$$\nu = \frac{\eta}{\rho}$$

The SI unit of kinematic viscosity is square meter per second (m^2s).

The viscosity curves of Fe-Ni and Cr-Ni systems at 1873 K and a comparison to experimental data are shown in [Figure 3](#).

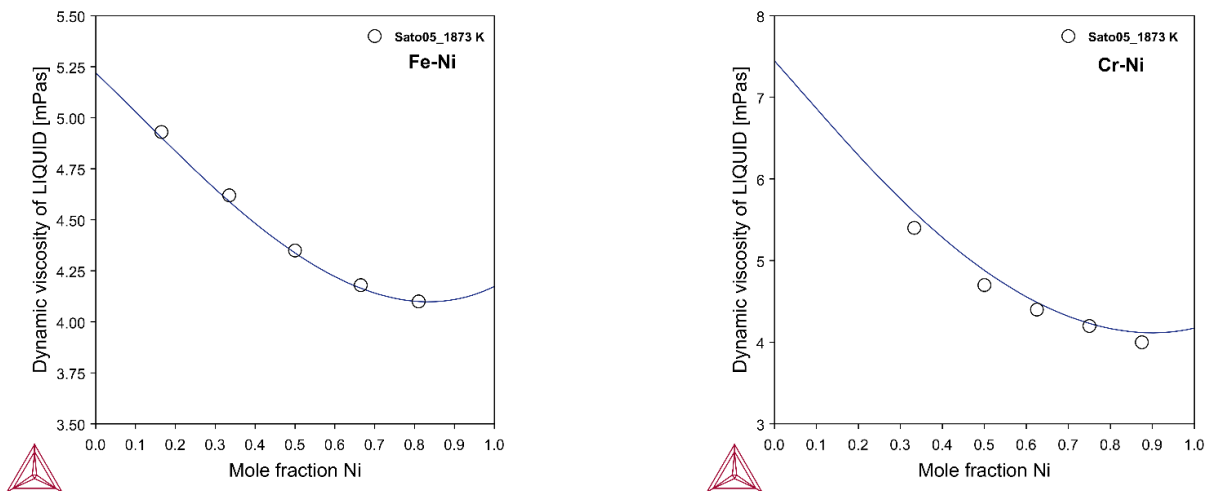


Figure 3: Isoviscosity curve for Fe-Ni system at 1873 K (left). Experimental data is from [2005 Sato] compared to isoviscosity curve of Cr-Ni system at 1873 K (right). Experimental data is from [2011 Sato].

The viscosity of Cr-Fe-Ni ternary system at 1800 K is calculated from assessed binary parameters and is shown in [Figure 4](#).

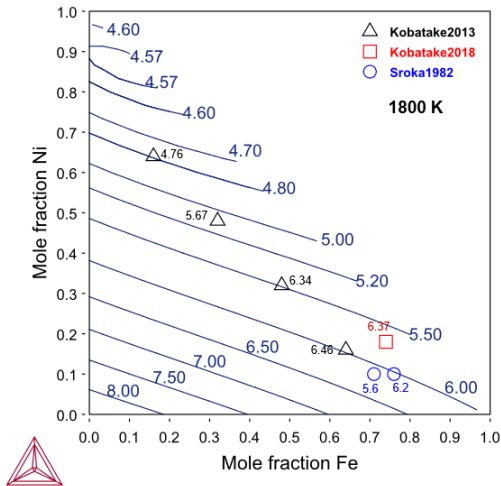


Figure 4: Isoviscosity of Cr-Fe-Ni at 1800 K. Experimental data is from [2013 Kobatake, 2018 Kobatake, 1982 Sroka].



In Console Mode, the viscosity can be plotted via a step calculation vs. temperature or composition. The relevant property is VISC of the liquid phase. The calculated VISC property is not the viscosity (η) but is related to η via $R * T * \ln * \eta$, thus in order to plot the viscosity or η , one needs to define a function for η as follows:

$$\eta = \exp(\text{VISC}(\text{LIQUID}) / (R * T)) \text{ [Pa.s]}$$



In Graphical Mode, the viscosity (η) is directly plotted via the one axis calculation type.

Ordered Phases

The ordered phases BCC_B2 and FCC_L12 are described based on the order/disorder partitioning model as described by Lukas et al. [2007].

In TCFE10 the disordered part of BCC_B2 and FCC_L12 (A2_BCC and A1_FCC respectively) are identical to the ordinary BCC_A2 and FCC_A1, but only 1 J/mole of formula unit less stable. This way the ordered phases BCC_B2 and FCC_L12 are split from the disordered BCC_A2 and FCC_A1, and the second order phase transitions are automatically displayed by a narrow first order transition ([Figure 5](#)).



No phase is rejected by default in the database.

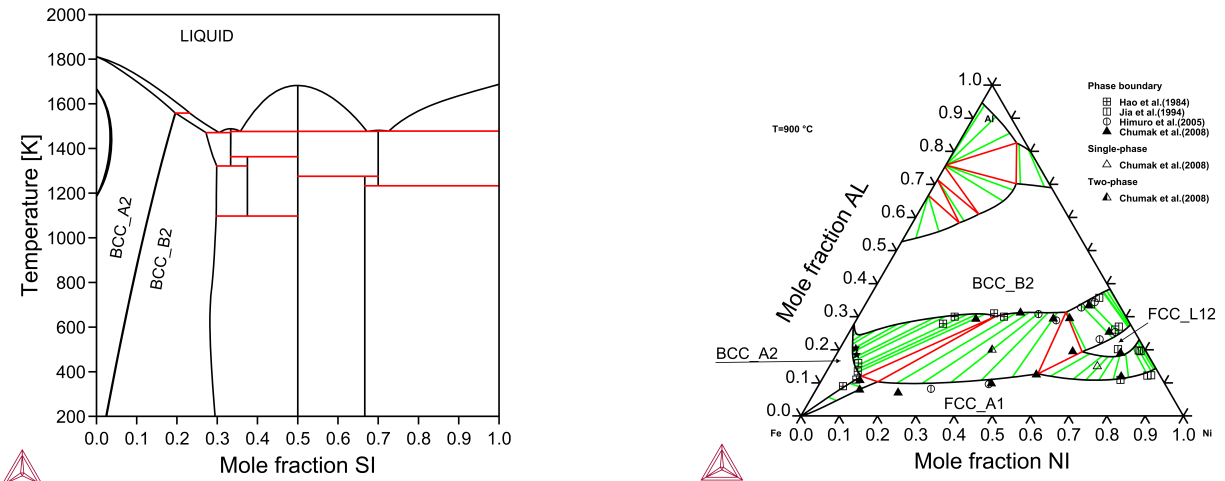


Figure 5: Fe-Si phase diagram (left) and isothermal section of Al-Fe-Ni phase diagram at 1273 K (right).