TCFE4: TCS Steel and Fe-alloys Database

Thermo-Calc Software is pleased to announce the release of TCFE4, a thermodynamic database for different kinds of steels and Fe-based alloys for use with the Thermo-Calc and DICTRA software packages. This release builds on the previous version of the database, i.e. TCFE3, and additionally includes a complete assessment of molar volume data for all phases typically present in steels.

The benefit from having molar volume data included in the database is the possibility to calculate and plot directly within Thermo-Calc:

- Volume fraction of phases.
- Volume for a phase or for the whole system.
- Density for a phase or for the whole system, see Fig. 2.
- Lattice parameters (for phases having cubic structures).
- Relative length change and thermal expansion coefficients, see Fig. 1.

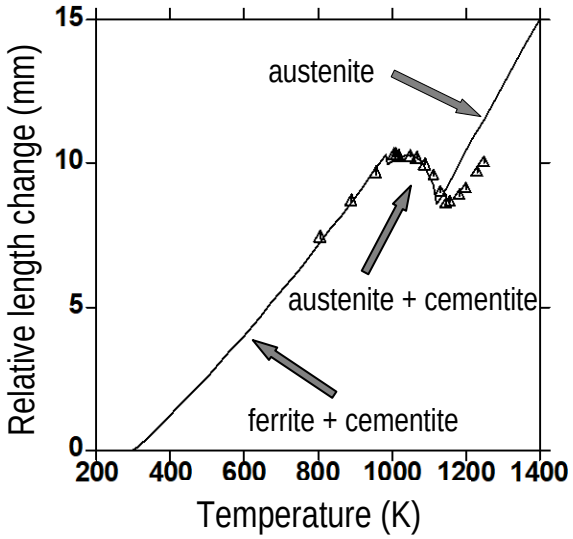

Fig. 1: Relative length change in a steel with 0.11%C-0.5%Mn-0.03%Si-0.01%Cr-0.02%Ni.

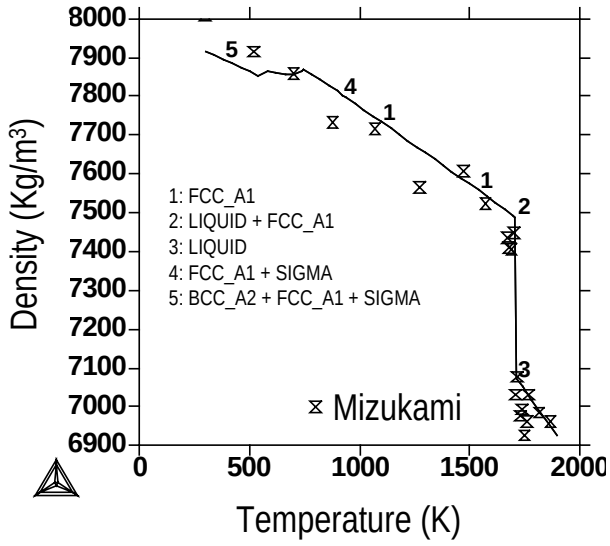

Fig. 2: Density for a Fe - 18.13%Cr - 25.55%Ni alloy vs. temperature.

Critically assessed phases are listed in the table below. All remaining phases are assigned reasonable default values for the volume at 298.15K, as well as for the integrated thermal expansivity.

Solution phases	Liquid*, fcc, bcc, hcp* (* Partially assessed)
Carbides	Cementite, fcc-carbide, M12C, M23C6, M6C, M7C3, SiC, Al4C3, B4C
Nitrides	fcc-nitride, AlN, BN(hP4)
Oxides	fcc-oxide, SiO2 (cristobalite, quartz, tridymite)
Complex compounds	Laves, Sigma, Mu-phase
Other phases	B2M, B3Si, Fe2Si, FeB, FeP, Graphite

The volume data now included in the databases is based on so-called CALPHAD assessments. Large amounts of experimental data ranging from binary to multi-component systems have been collected and critically assessed. In order to keep the database consistent, experimental data for higher-order systems have also been taken into consideration during the assessment of lower order systems. This method also allows reasonable estimates for metastable phases to be accomplished. For metastable phases, Ab-initio calculations were also performed in order to calculate molar volumes at T=0K. The Debye-Grüneisen model was in these cases used in order to predict thermo physical properties at finite temperatures.

Figures 3-6 below provide examples of calculations now possible using the new database and Thermo-Calc.

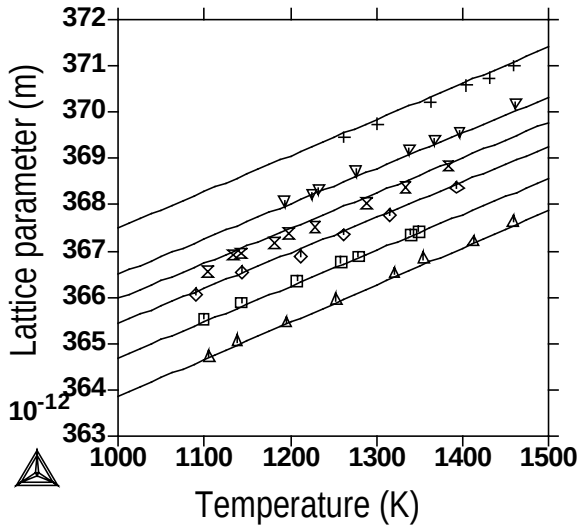

Fig. 3: Calculated lattice parameter for Fe-C alloys (0.32 – 1.44 %C) vs. Temperature. Symbols are experimental data from Ridley.

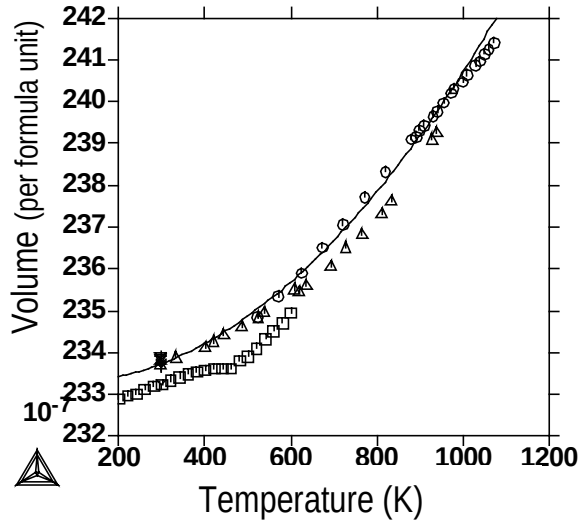

Fig. 4: Calculated volume (per formula unit) of cementite in comparison with experimental data.

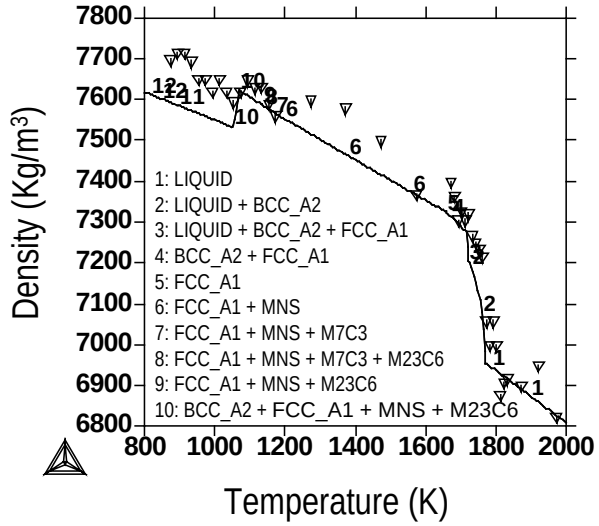

Fig. 5: Calculated density for a Fe - 8.91%Cr - 0.2%C - 0.22%Si - 0.90%Mn - 0.011%P - 0.001%S alloy vs. temperature. Symbols are experimental data from Mizukami.

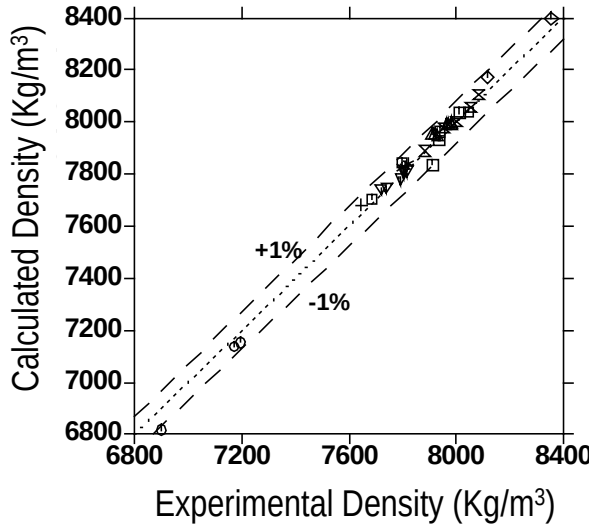

Fig. 6: Comparison of calculated and experimentally determined density at room temperature. Data points correspond to carbon steel, austenitic, ferritic and duplex stainless steels.