TCFE5: TCS Steel and Fe-alloys Database

Thermo-Calc Software is pleased to announce the release of TCFE5, 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 to the previous version of the database, i.e. TCFE4, and additionally includes complete reassessments of several binary and ternary systems performed under a three year collaborative program within the framework of the CCT-Applied project for stainless steels. CCT (Centre of Computational Thermodynamics) is a collaborative effort between the Royal Institute of Technology (Stockholm, Sweden), Kimab and Swedish industries.

Some of the major improvements to the TCFE5 database include improved thermodynamic descriptions for the following ternary and quaternary systems:

C-Cr-Si

- ✓ Cr-Ni-N
- ✓ Fe-Cr-Cu
- ✓ Fe-Cr-Si
- ✓ Fe-Ni-N
- ✓ Fe-Ni-Si
- ✓ Fe-Cr-Mo-C
- ✓ Fe-Cr-C-N
- ✓ Fe-Cr-Mn-N
- ✓ Fe-Cr-Mo-N
- ✓ Fe-Cr-Ni-N
- ✓ Fe-Cr-Si-N
- ✓ Fe-Cr-Ni-Al
- ✓ Nb-V-C-N

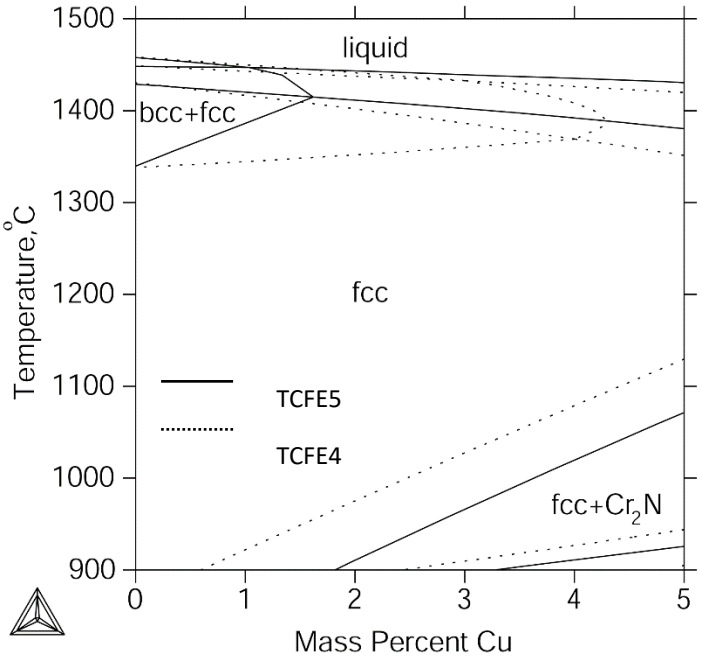

Fig. 1: Calculated phase diagram for increasing Cu content for a stainless steel using the TCFE5 and TCFE4 databases.

Validation of the TCFE5 database against experimental data shows that the new database is more accurate for predictions of:

Steels alloyed with N, especially the solubility of N in the liquid phase and the stabilities of the nitrides formed.

The relative stability between the austenite and ferrite phases in Al and Cu-rich alloys. Figure 1 demonstrates the improvement for a commercial alloy containing 2% of Cu, and it can be clearly seen that in the previous description the bcc phase was much more stable. This new thermodynamic description is verified from recent experimental information.

The relative stability between the austenite and ferrite phases in alloys containing Al, Cr and Ni.

Commercial alloys with high Si and Cr concentrations. Figure 2 shows for example a comparison of calculated liquidus temperatures, for commercial alloys having high Si and Cr contents, compared with experimental data. Additionally, the correct primary phase is now predicted to form from the liquid.

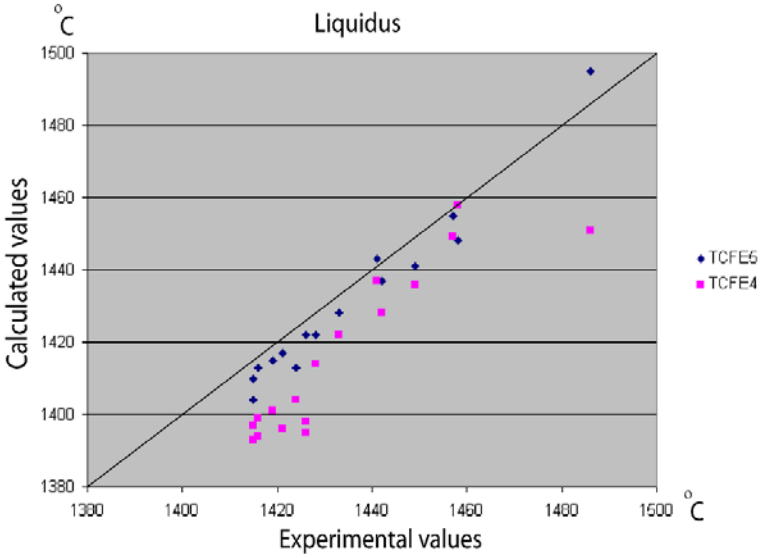

Fig. 2: Experimental liquidus temperatures of commercial alloys with high Si and Cr contents compared to calculations using the TCFE5 and TCFE4 databases.

Figure 3 demonstrates that TCFE5 still, in general, predicts the liquidus temperature well for different types of steels.

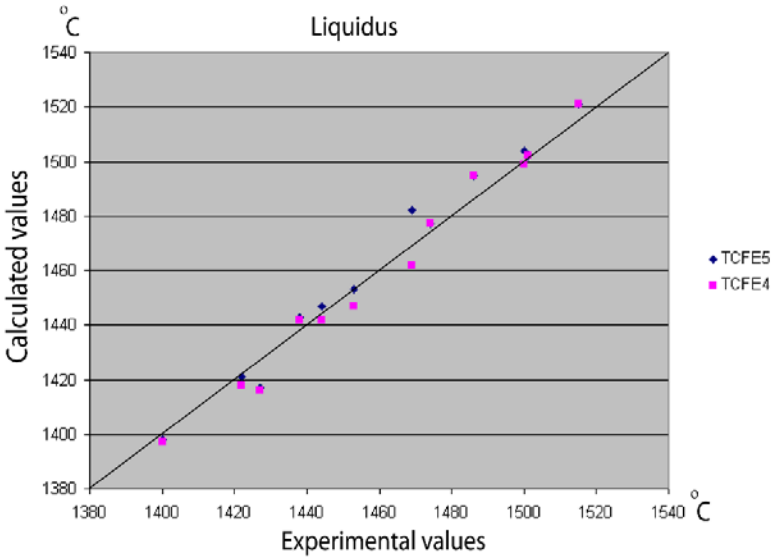

Fig. 3: Experimental liquidus temperatures for various steels (stainless steels, carbon and low alloy steels, high-speed steels and Chromium steels) compared with calculations performed using the TCFE5 and TCFE4 databases.

In addition, improvements in the Fe-Cr-Mo-C system together with models that predict the miscibility gaps between NbC-VC and NbN-VN will somewhat enhance the predictive capability for tool steels/high-speed steels and HSLA steels.

TCFE5 contains molar volume data for all phases in the database (introduced in TCFE4), which allows for the calculation of volume fraction of phases, as well as density and thermal expansivity using Thermo-Calc.