Thermodynamics and Properties Software

Thermo-Calc

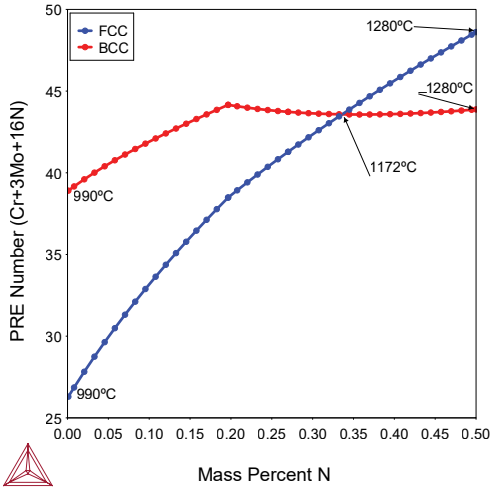
Thermo-Calc is used by materials scientists and engineers to generate material properties data, gain insights about materials, understand a specific observation, and answer direct questions related to a specific material and/or its processing. The software platform includes several built-in calculators that allow you to perform a wide range of thermodynamic and property calculations. It can be expanded with Add-On Modules to make many other calculation types.

Predict a Wide Range of Materials Property Data

Below are examples of properties that can be calculated with Thermo-Calc, typically as a function of composition, temperature, and sometimes also pressure:

- **Thermophysical properties:** Specific heat, enthalpy, heat capacity, heat of formation, density, coefficient of thermal expansion, viscosity (of liquid), surface tension (of liquid), interfacial energy, thermal conductivity, electric resistivity
- **Kinetic properties:** Diffusion coefficients, atomic mobility
- **Mechanical properties:** Yield strength, hardness
- **Properties related to equilibrium and non-equilibrium solidification:** Liquidus, solidus, incipient melt temperatures, freezing range, fraction solid curves, solidification path, fraction eutectic, microsegregation, partition coefficients, latent heat, shrinkage, susceptibility to hot tearing, and more
- **Properties specific to steel:** Martensite start temperature, martensite fractions, and kinetics of pearlite, bainite, and ferrite formation
- **Properties specific to nickel:** Antiphase boundary energy, coarsening, and equilibrium with freeze-in temperature

**Requires a license for the Steel or Nickel Model Library*

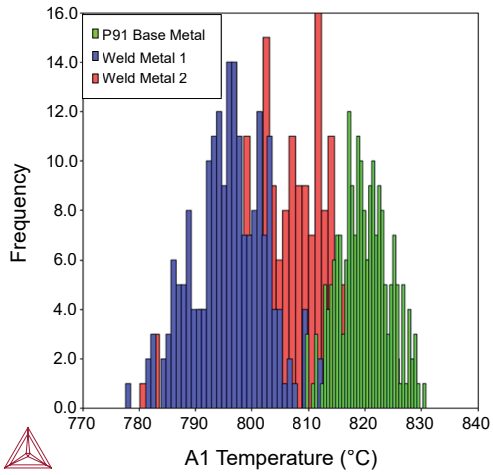


Calculated PRE (pitting resistance equivalent) for ferrite and austenite in a 2507 duplex stainless steel. When the alloy has 0.33wt% N, the PRE is equal in both phases, which helps avoid preferential corrosion. The homogenization temperature required to get a balanced 50/50 microstructure is shown to be 990 °C – 1280 °C with 1172 °C providing the optimal equivalent PRE.

Gain Insight into Materials Processing

Simulations can be used to gain insight into how to optimally process an alloy. There are numerous applications of how Thermo-Calc can be applied to this topic, including but not limited to:

- Optimizing slag systems for both ferrous and non-ferrous applications
- Calculating furnace gas chemistries
- Predicting microsegregation following processes involving solidification
- Identifying optimal temperatures for solutionizing, homogenization, annealing, and more
- Predicting precipitate phases to form during heat-treatment
- Predicting the time needed to homogenize segregations (requires the add-on Diffusion Module (DICTRA))
- Simulating the growth/dissolution time of precipitates (requires the add-on Precipitation Module (TC-PRISMA))



Histogram showing the A1 temperature calculated for 200 compositions each that fall within the P91 base metal and two weld filler metal matching composition specifications. As can be seen, if the post weld heat treat temperature is selected according to the base metal compositions, the A1 temperature could be exceeded in the weld metal resulting in fresh martensite formation.

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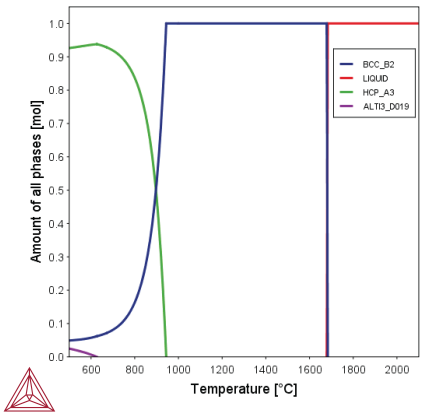
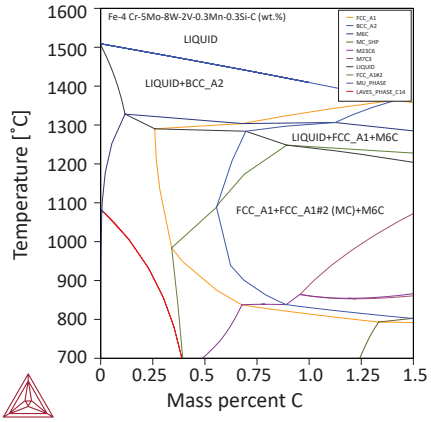
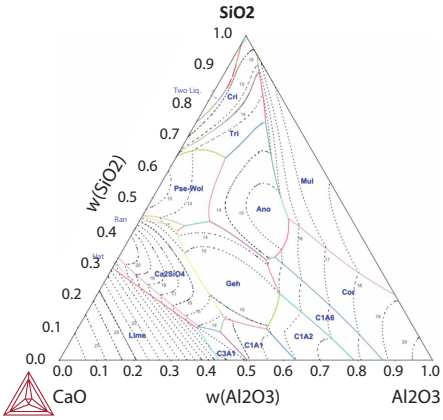


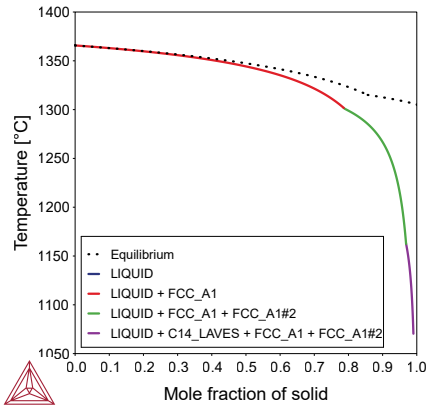
Stable phases vs temperature for Ti-6Al-4V



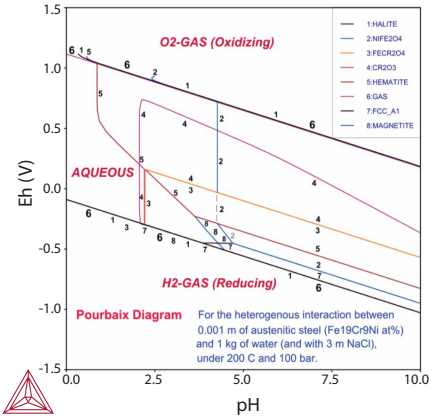
Mapped diagram for M42 high speed steel



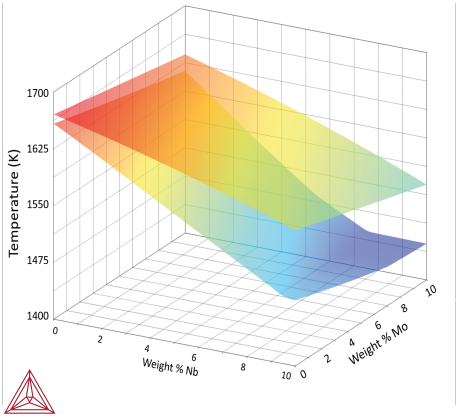
Ternary liquidus projection in oxide systems



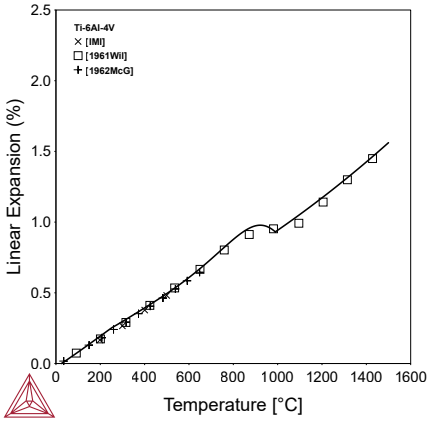
Scheil Solidification Simulation of Ni-base alloy 625



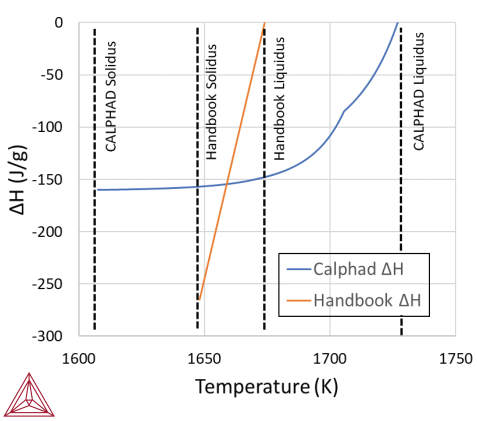
Pourbaix diagram for austenitic stainless steel



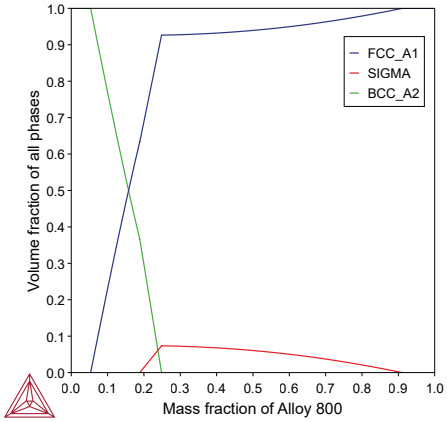
3D Liquidus and Solidus vs Nb and Mo wt% in Ni Alloy 718



Linear expansion vs temperature for a Ti-6Al-4V composition compared with experimental data



Calculated latent heat compared to handbook values for 316L



Gradual transition from a martensitic stainless steel (left) to Alloy 800 (right) at 650 °C