The SPREFR Database for refractory systems with Carbide, Nitride, Boride and Silicide Phases

The SpencerGroup 2013
(supported by GTT)

Scope of the *SPREFR* database

- Relates to the ever-expanding field of *non-oxide refractories* based on carbides, nitrides, borides and silicides.

- Applications: hard, high melting temperature materials used in *furnace construction, high-temperature coatings, cutting tools, abrasives, aircraft brake linings, rockets, jets, turbines,* and *nuclear power plants.*
- Also as *precipitates* in *steels* and *light alloys* to give improved properties through added strength, hardness, and grain refining. (Combine with ***FTLite*** and ***FSStel***)

Further aspects

- **Reactions** of the carbide, nitride, boride and silicide systems **with refractory oxides** and **oxygen-containing gases** can be calculated by *combining* the ***SPREFR*** database together with such databases as ***FToxid***, ***FACTPS*** and ***SGPS***.

Component list

- ***B, C, N, Si*** with
- combinations of **Al, Ca, Co, Cr, Fe, Hf, Mg, Mn, Mo, Nb, Ni, Re, Sc, Ta, Tc, Ti, V, W, Y, Zr**

Database contents

- Assessed thermodynamic parameters for binary and ternary systems
- Major subsystems: Me1-Me2-C, Me1-Me2-N, Me1-Me2-B, Me1-Me2-Si, Me-C-N, Me-C-B, Me-C-Si, Me-N-B, Me-N-Si and Me-B-Si
- Total number of systems: appr. 180 binary, and over 200 ternary systems
- Total number of phases: 311 solutions and appr. 470 stoichiometric compounds

Data assessment/generation

- Combine available assessed thermodynamic data for the appropriate binary sub-systems with the phase boundary information contained in the ASM Handbook of Ternary Alloy Phase Diagrams

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completely compatible set of parameter values to describe binary and ternary thermodynamic properties and phase equilibria for a particular system

Data assessment/generation ctd.

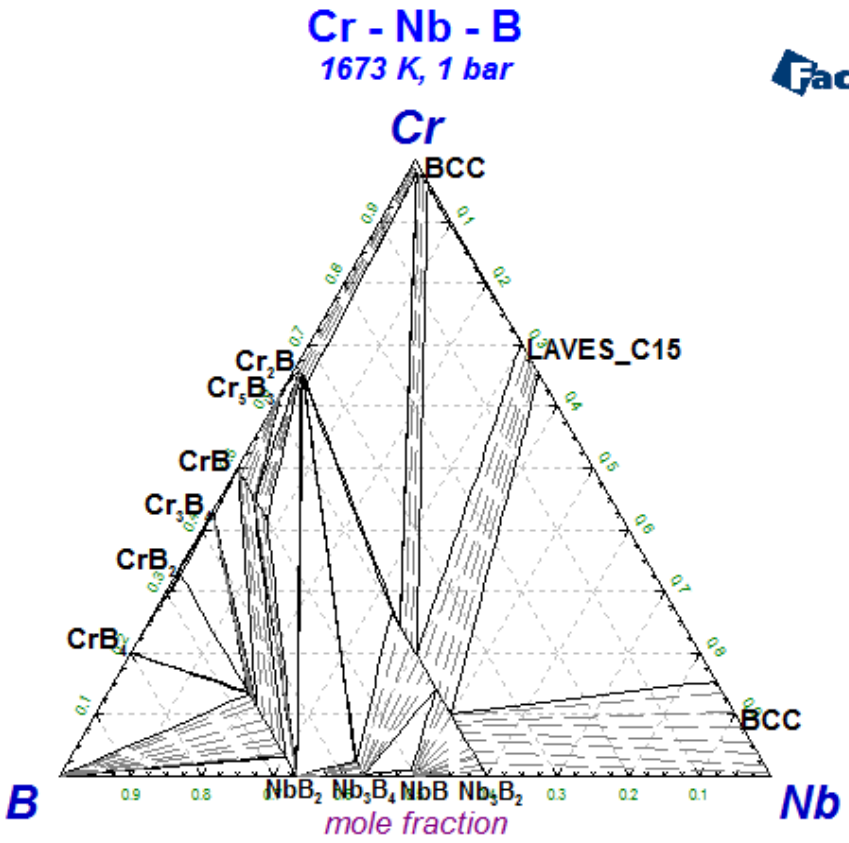
- Great scarcity of published experimental thermodynamic values for the phases of ternary systems → additivity of element entropy and heat capacity data assumed frequently (Neumann-Kopp)
- Enthalpies of formation and standard entropies of the compounds derived to give consistency with the published phase equilibria

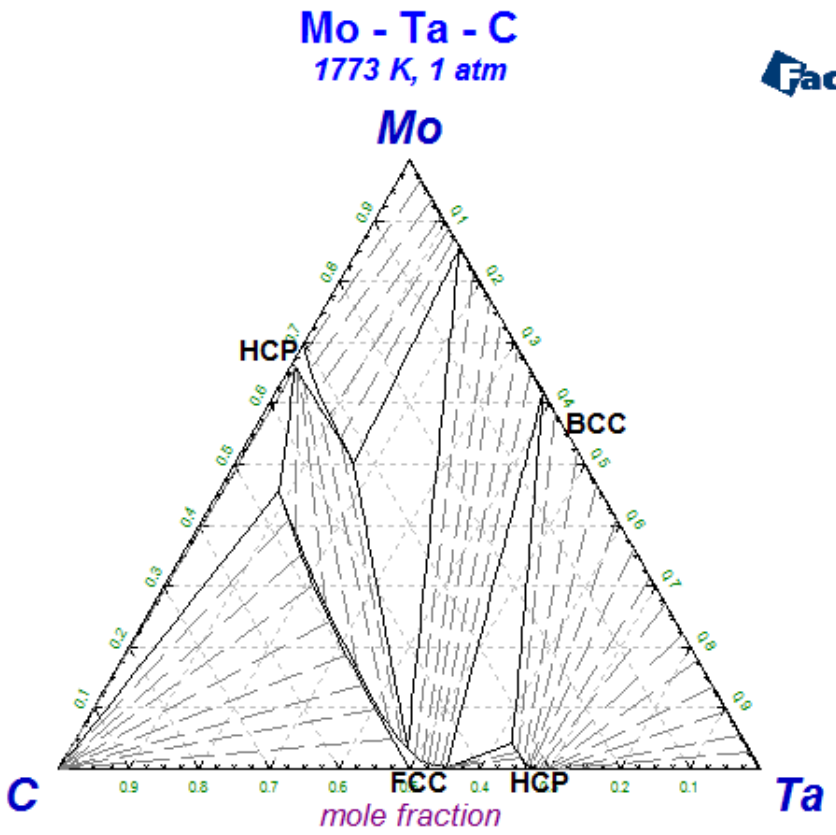
Gibbs Energy models used

- Liquid: Substitutional solution of the elements → Redlich-Kister-Muggianu
- Solid compounds: classical G-function based on H_{298}, S_{298} and $c_p(T)$
- Solid solutions: Multi-sublattice model, i.e. Compound energy formalism

Phase Diagram Examples

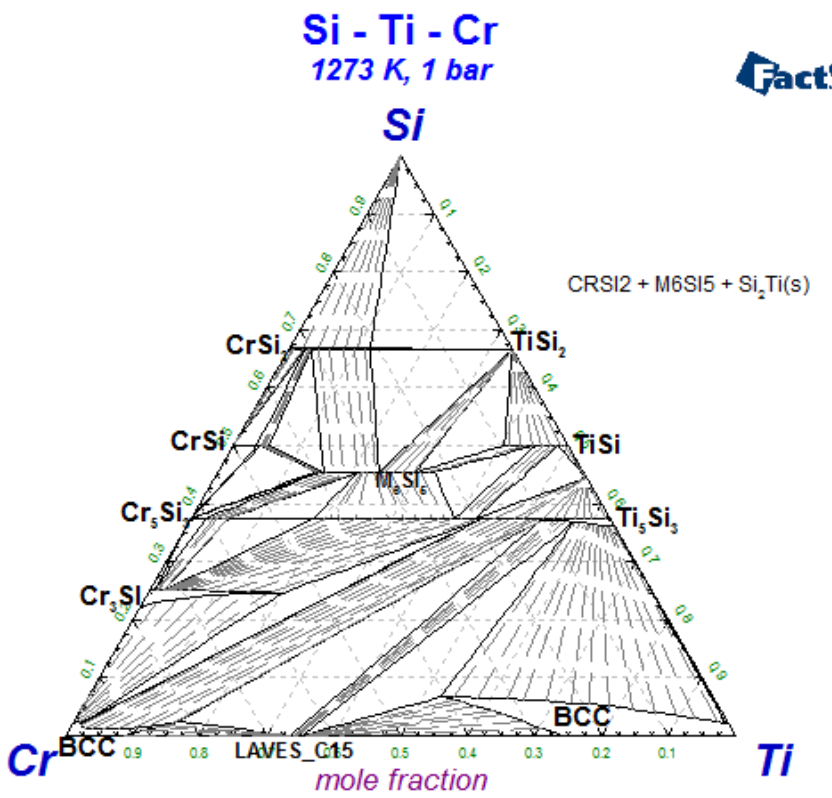
two metal - boride, two metal - carbide

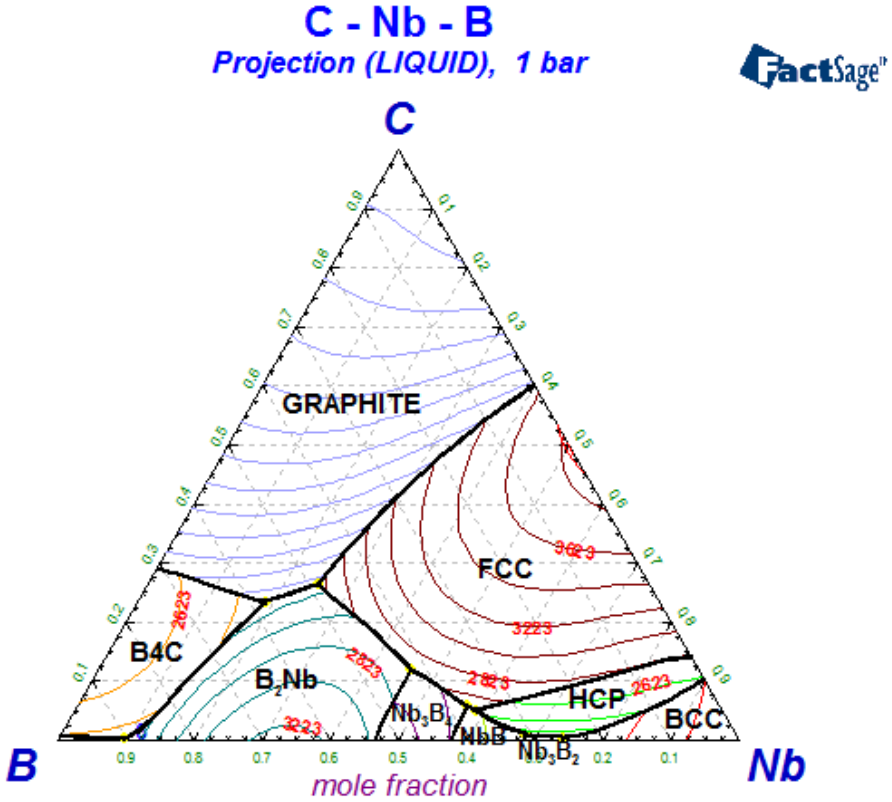




Phase Diagram Examples

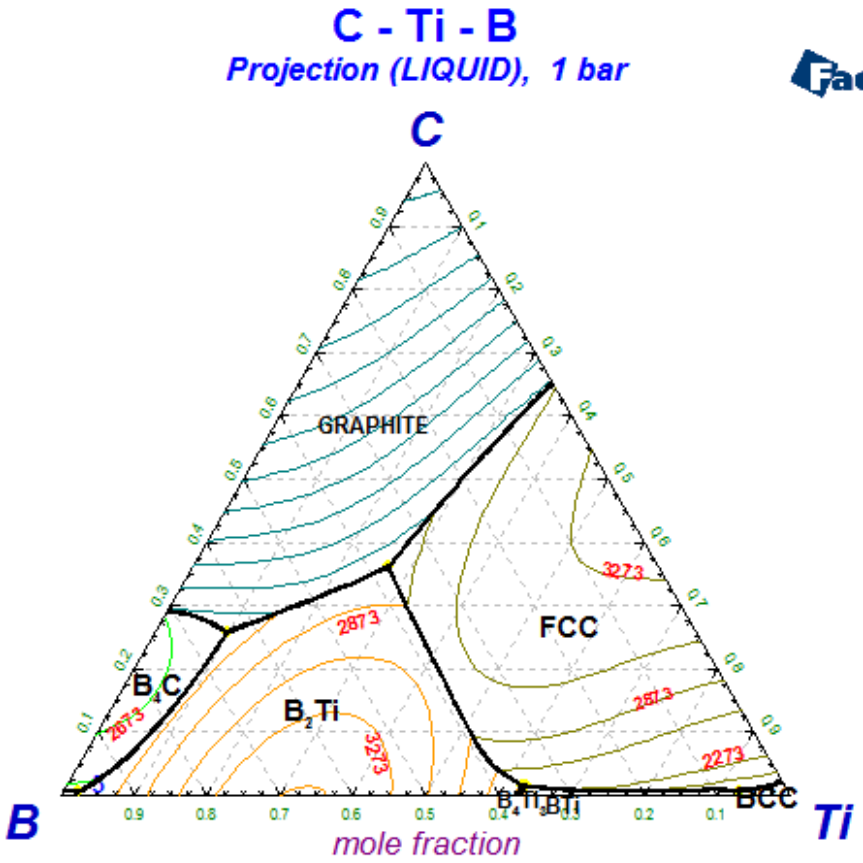
two metal - silicide, one metal - C+B

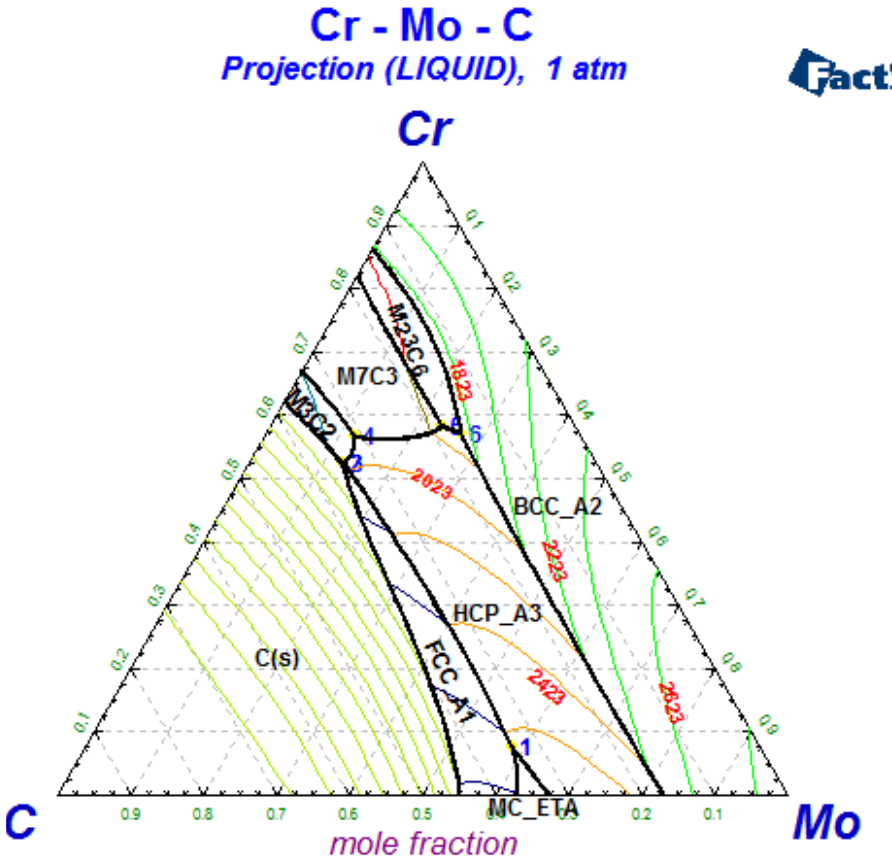




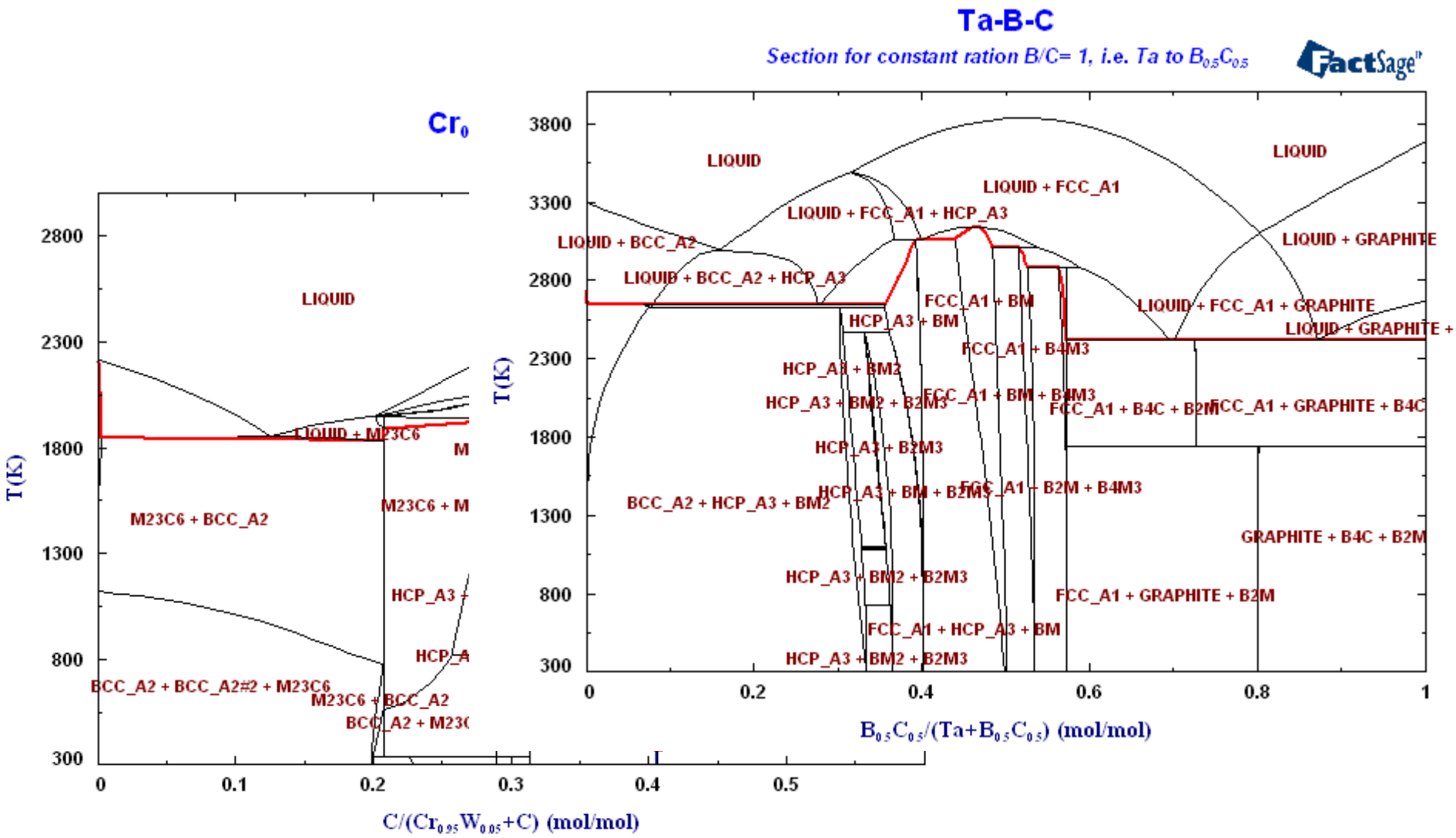
Phase Diagram Examples

one metal - C+B, two metal - carbide





Vertical sections



Thank you for your attention !