Database Description:

Thermodynamic Database for Hardmetals ICEM_2

The ICEM_2 thermodynamic database describes the alloy system Co-Ta-Ti-W-Zr-C-N. It is an extension of the ICEM database (Co-Ti-W-C-N) by adding the alloying elements Ta and Zr. It is valid for calculations of phase equilibria in hardmetals with a Co-binder and containing WC. This means that it provides a good description of the phase equilibria between a solid or liquid Co-rich binder phase (liquid/fcc) and WC; M6C carbides; graphite; and cubic carbides/nitrides/carbonitrides.

Thermodynamic descriptions of several lower order systems are implemented in the database, for details see the reference list at the end of this document. The database is not simply a collection of lower order systems. It is validated towards specific applications and will therefore be accurate to obtain:

- Melting temperatures of the Co binder
- Carbon windows (allowed C-content where M6C carbides and graphite are avoided)
- Composition of the mixed cubic carbides/nitrides/carbonitrides (Ta,Ti,W,Zr)(C,N) under varying conditions
- Composition of the liquid and solid Co-binder (in equilibrium with WC + other carbides)

Some of the lower order systems in the database are included with simplified descriptions (for example Co-Ti), and more recent assessments may be available. If you substitute these descriptions, you should make sure to check the calculations of the properties listed above so that the predictions are still reasonable. The descriptions of the binary alloy systems can be critical.

<u>Addition of Ta</u>

The database involves a full description of the Ta-C and Ta-N binary systems, thereby providing the thermodynamic properties of the Ta-carbides and Ta-nitrides. A description of the Ta-C-N system determines to what extent the carbides and nitrides are soluble in each other.

A full assessment of the Ta-W-C system is included in the database. This system is important since its thermodynamic description determines how much W that is solved in the Ta-carbide. This solubility has been measured, and the experiments are well described. The solubility of W in (Ta,W)C is important for applications to hardmetals, since it affects the amount of W that remains to form the WC-phase. Calculations are valuable to balance compositions to obtain the phases that are aimed for, and in correct amounts.

The effect of nitrogen in Ta-W-C-N was investigated in [12] by calculations, showing that Ta, similarly to Ti, will diffuse from the surface when a nitrogen containing hardmetal is sintered in nitrogen free atmospheres. Calculations can be a valuable guide to optimize compositions and predict gradients.

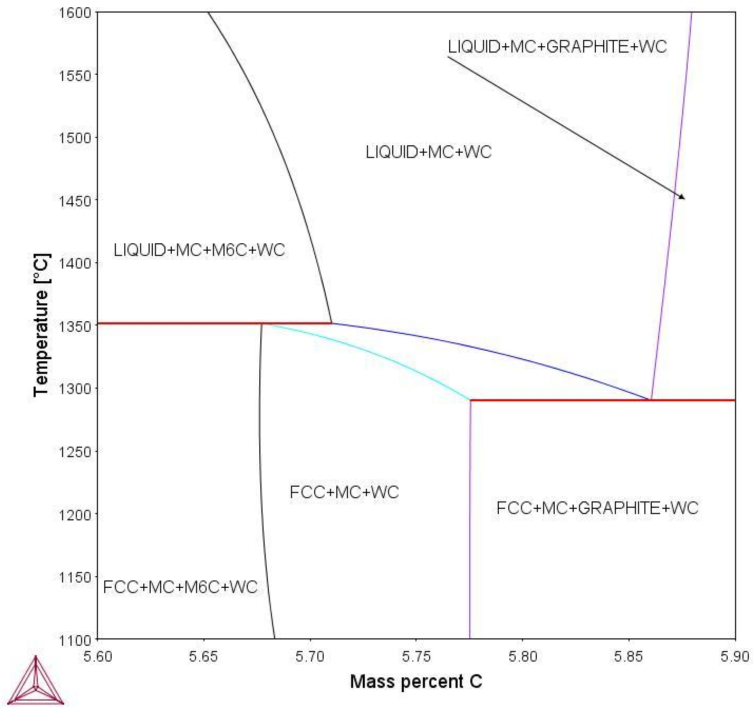
Another critical information for hardmetal applications is the melting temperature of the binder in various alloys. To provide consistent experimental information measurements of the melting temperatures of alloys with a Co-based binder and a C-content determined by the presence of WC; M6C; graphite; and cubic carbides; were performed [10]. A few alloy systems in the database were adjusted to this information to get good agreement:

- The thermodynamic parameter for the liquid phase in the Co-Ta-W system has been adjusted to the melting temperature experiments. The Co-Ta-W system is described in the Co-rich corner. This means that you should not use this database for predictions in the low Co region.
- A description of the liquid phase in the Co-Ta-C system was obtained based on the melting temperature measurements.

Cubic carbonitrides are important consitutents for hardmetals with nitrogen. In the sublattice model that is used for the thermodynamic descriptions, miscibility gaps are often predicted and can need adjustments. Parameters were therefore introduced in the quaternary fcc phase in the Ta-Ti-C-N system.

Application Example

The balance of C to obtain Co(fcc)+WC+MC(cubic carbide), without detrimental carbides (M6C or graphite), often called carbon window, can be calculated. The figure below shows the carbon window for a 6wt%Co-0.84wt%Ta-W-C material. The composition of "MC" is the cubic carbide (Ta,W)C. At a sintering temperature of 1350°C the carbide is predicted to dissolve 11wt%W. Several reports show that the addition of Ta to Co-W-C hardmetals decreases the grain growth of WC due to the partitioning of W between WC and (Ta,W)C. This leads to improved microstructures and properties.



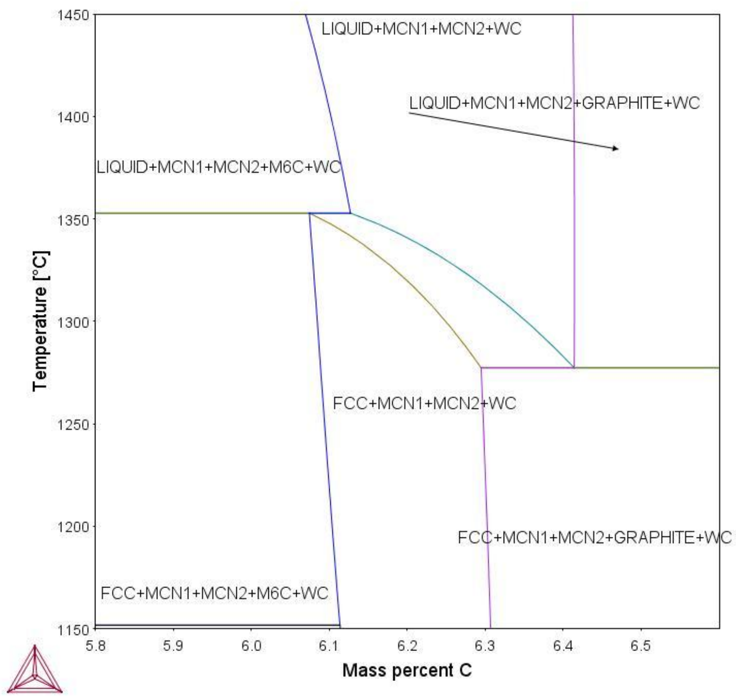
Addition of Zr

A full description of the Zr-C and Zr-N systems are included in the database. Further, the Co-Zr, Ta-Zr, Ti-Zr, W-Zr, Co-W-Zr, Ti-Zr-C, W-Zr-C, Zr-C-N, and the Co-Ti-W-Zr-C systems have been implemented.

In alloy systems with several cubic carbide/nitride formers a miscibility gap is predicted. To be able to describe these materials control of the miscibility gaps is needed. For this purpose, experiments were made in [93]. These data were used to adjust thermodynamic parameters.

Application Example

A calculated diagram for the composition 8wt%Co-3wt%Ti-0.2wt%N-3wt%Zr and a varying C content is shown below, illustrating the C-window for this composition. The carbonitrides separate into two different compositions: MCN1 - (Ti,W,Zr)(C,N) and MCN2 - (Zr,W,Ti)(C,N). This has also been verified experimentally in different reports in the open literature. Above 1460°C the miscibility gap closes when calculated with the ICEM_2 database.



Data for molar volumes and thermal expansion

Data for molar volumes and thermal expansion are included in the database so that volume fractions of the various phases can be calculated. The predicted volume fractions are expected to be accurate. However, some data has been estimated, especially the thermal expansions. If you want to use this data for detailed calculations, please validate the data.

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