CALPHAD assessment of the Ti-W system including experimental and ab-initio data

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Motivation

The Titanium-Tungsten phase diagram was previously assessed by Jin [1993] [1] and Jonsson [1996] [2]. These assessments were based solely on experimental data, which is rather scarce, especially at low temperatures (< 1373 K), where the only information is the solubility of W in the Ti-rich HCP phase and the temperature and composition of the eutectoid point. Recent density functional theory calculations [3], [4] show that the DFT mixing energy of the BCC phase at 0 K deviates largely from the mixing enthalpy predicted by the thermodynamic database (TDB) of Jonsson.

We propose a new assessment of the Ti-W thermodynamic database, by combining experimental and density functional theory data including all three stable phases (BCC, HCP, liquid). The optimization of the TDB parameters is done with the python based open source programs pyCalphad [5] and ESPEI [6].

Conventional Ti-W phase diagram

The Ti-W phase diagram (PD) after Jonsson [2] (figure on the left). The Ti-W system shows three stable phases: BCC (α), HCP (β) and Liquid (L) and in particular:
- Miscibility gap of BCC Ti and BCC W with the critical point at X(W) = 0.39 at% and T = 1533 K
- Low solubility of W in HCP(Ti) (0.2 at%)
- Eutectoid point at 9.6 at%, T = 1018 K
- Two phase region of HCP(Ti) and BCC(W) below 1018 K
- Extrapolation of miscibility gap below 1373 K is uncertain (no data points)

Redlich-Kister parameters of Jonsson:
- BCC: 1st order interaction parameters, no T-dependence
- HCP: 0th order interaction parameter, no T-dependence
- Liquid: 0th order interaction parameter, no T-dependence

New data from ab-initio

- DFT mixing energies for BCC deviate largely from prediction from the interaction parameters of Jonsson
- Conventional phase diagram is erroneous at low temperatures and high W content
- Solubility of Ti in BCC(W) at low temperatures should be > 20 at% due to strong negative mixing energy

New Phase Diagram

Parameter optimization with ESPEI [5]
- Low Temperature region is different and should be described better
- Solubility of Ti in BCC(W) is approximately 25 at% at 300 K
- Eutectoid point shifted to lower T and higher X(W) (similar to [3])

ESPEI optimization with Markov Chain Monte Carlo gives parameter-set distribution which allows for uncertainty estimation:
- (α+β/β) phase boundary distribution from parameter-set distribution:
  - Reduced uncertainty in position of the phase boundary at 300K (b) compared to the ESPEI optimization without the mixing energy (a)
  - Eutectoid point varies between T = 800-980 K and X(W) = 0.9-0.16 at% between different parameter sets -> further clarification needed

Conclusions

- We propose a new assessment of the Ti-W system including all three stable phases using experimental and DFT data.
- High solubility (> 20 at%) of Ti in BCC(W) at 300 K due to strong negative mixing energy at W rich side.
- Further experiments at low temperature required for clarification.

References: