WEBINAR

Questions & Answers

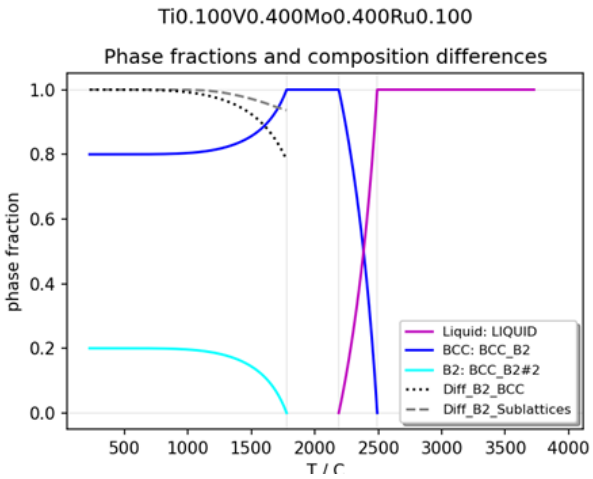
High-Throughput Exploration of Refractory Superalloys with Experimental Verification

Presenter: Dr. Sebastian Kube

This is a collection of questions that were not answered live during the webinar and are not included in the recording.

Q1: At slide 20, what is two kind of BCCB2 phase in the curves?

On slide 20 the cyan-colored curve represents the B2 phase fraction, and the dark blue-colored curve represents the BCC phase. We also self-calculated two additional curves: The dotted curve “Diff_B2_BCC” represents the compositional difference from 0 to 100at.% between the BCC and the B2 phase, and the dashed curve “Diff_B2_Sublattices” represents the compositional difference in at.% between the two B2 sublattice compositions as predicted by TC.



Q2: What about the price of an alloy with 15%Ru?

Indeed, Ru is hard to beat for high temperature stability, but unfortunately the cost of Ru significantly increased while we were conducting this research project. For commercially more viable alloys, we are currently working on modified alloy systems with reduced or substituted Ru contents.

Q3: How accurate (relatively) has DICTRA been for simulating the homogenization schedule for annealing out dendrites / dissolving secondary phase? Orders of magnitude similar for the given temperatures?

Answer from Thermo-Calc Software: Sebastian did not use DICTRA simulation in this work, but the Thermo-Calc team of application specialists would be happy to help provide a demonstration of DICTRA capabilities on this topic. You can contact us at info@thermocalc.com.

Q4: Nice talk! How do you think about the DBTT problem in your design?

We have been using different metrics to estimate ductility at RT ahead of time. However, this is a difficult property to predict especially in these complex multiphase RMPEAs systems. Therefore, we experimentally screen our alloys, primarily through compression testing at RT and 1200C (should be published a few months from now). Our starting strategy is to find ductile single-phases that can serve as a good matrix base.

Q5: Wonderful talk! How long would it take to assess one matrix-precipitate pairing (setup and run-time)?

Calculating one temperature curve for a given composition typically took us 30 secs. Calculating multiple compositions across the ternary or quaternary B2-matrix paired alloy systems therefore typically took up to 5 mins.

Q6: Could you throw some more light on how did you tackle the problem of microstructure inversion that is B2 as matrix?

In our analysis we used as default composition 30% B2 elements and 70% BCC matrix elements. So just considered from relative fractions, the BCC phase has a higher chance to form a continuous matrix phase. Also, we focused on systems predicted by TC to solidify first as BCC, and then precipitate B2 at a lower temperature. These are the systems color-coded in dark-blue in our large space maps (slide 21 and following). Meanwhile, we avoid systems predicted to solidify first as B2, and then form a coexistent BCC phase, which are color-coded in light-blue in our maps.

Q7: Thanks for the nice presentation. I wondering which experiment you have carried out to solutionize your materials at dry high temperature for eg 1600C

See methods details in our publication: https://doi.org/10.1016/j.actamat.2023.119628.

Q8: How do you account for impurities in the high Throughputs modeling? OR, how much do those impact the results?

In our analysis we assume high purity feedstock materials used in our experiments. We do not seem to have major issues with this approach. Avoiding oxidation and contamination with N and C is of course a major challenge, can lead to the formation of oxide phases etc. and in some cases significantly affect mechanical properties. In cases where we observed severe oxidation, we redid experiments. We also performed interstitial analyses to verify that our C,N,O contents are at typical low levels, see details in SI of our publication: https://doi.org/10.1016/j.actamat.2023.119628.

Q9: Also, to your knowledge, what are the highest solidus and highest solvus, individually solidus only and/or solidus and solvus highest refractory designed and proven out?

See predicted solidus and solvus temperatures (including high resolution images of the BCC-B2 space maps) and experimental temperature ranges determined in our publication and SI: https://doi.org/10.1016/j.actamat.2023.119628.

Q10: Where do you find the molar volumes data?

For lattice constant calculations, we used DFT data from the Open Quantum Materials Database (OQMD) for both BCC and B2 phases, which allowed us to account for non-additivity in the bonding. See also details explained in the SI of our publication: https://doi.org/10.1016/j.actamat.2023.119628.

Q11: I see TC has the Nickels TDB which has Oxygen gas phase etc. And TC advertises the TCOX oxides /slag ...are these useful?

Answer from Thermo-Calc Software: The TCNI database has a limited subset of oxides applicable mainly to Nickel-base superalloys. Furthermore, TCNI has a complete GAS phase description, which makes it compatible with the Additive Manufacturing module.

The TCOX database has a more elaborate description of the oxides and other slag materials. So which database to choose, it depends on what you want to use it for! Feel free to contact us for more information, at, info@thermocalc.com.

Q12: Can the exploration of the BCC system like this work result in cuboidal precipitates like the Ni based alloys?

Some of our microstructures do exhibit sub-micron precipitate particles, which in some cases we have confirmed to be coherent by TEM, and which often show some degree of cuboidal geometry. Achieving a cuboidal geometry just as in Ni-based superalloys will require more optimization work. As one example, stay tuned for a study led by my colleague Carolina Frey, which achieved beautiful cube-on-cube precipitation morphologies (should be publicly available in a few months).

Some attendees asked about open PhD and Postdoc positions. You can contact Dr. Sebastian Kube for information about available positions by emailing Sebastian.Kube@wisc.edu.