56-L.0 THERMOMECHANICAL PROCESSING OF REFRACTORY MULTI-PRINCIPAL ELEMENT ALLOYS FOR ULTRAHIGH TEMPERATURE PERFORMANCE

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56-L.1 Project Overview and Industrial Relevance

Refractory multi-principal element alloys (RMPEAs) are a relatively new class of alloys that show potential for withstanding continued operation at elevated temperatures [56-L.1]. RMPEAs are of particular interest for replacing modern nickel- and cobalt-based superalloys in ultra-high temperature applications, such as jet turbine engines, because modern superalloys have limited operability above 1100°C and require coatings and coolant systems which reduce efficiencies. RMPEAs with higher operational temperatures have the potential to improve component lifetimes and engine efficiencies [56-L.2].

This project will focus on developing thermomechanical processing methods to control the microstructure and properties of selected RMPEAs, with the goal of identifying deformation mechanisms and building processing maps. The effect of interstitial carbon and oxygen will also be investigated to determine deleterious or beneficial effects, such as precipitation strengthening and/or grain size control. Alloy and microstructural design will also be considered.

56-L.2 Previous Work

The field of RMPEAs is still relatively immature. Some early studies indicate that, while multi-phase RMPEAs are typically stronger than single-phase RMPEAs at room temperature, single phase RMPEAs may maintain their strength better at elevated temperatures [56-L.3]. Previous work has been done to develop an improved solid solution strengthening model for predicting the athermal and thermally activated components of yield stress for RMPEAs, TC-EARS [56-L.4]. This model, along with Thermo-Calc CALPHAD simulations, are being used to identify compositions with high athermal yield stress and single-phase structures.

The effect of interstitials on properties and microstructure development of RMPEAs has not been fully explored, but, historically, commercial refractory alloys have been studied in the context of interstitial additions. The Nb alloy WC-3009 has oxygen additions that form stable Hf oxides and exhibits significantly improved oxidation resistance compared to other Nb alloys [56-L.5, 56-L.6]. The presence of Hf to form oxides may prevent deleterious effects from oxygen interstitials, but this effect is not yet well studied in RMPEAs. Some conventional Ta-based refractory alloys, such as ASTAR-811C, use carbide dispersions to improve high temperature strength and creep behaviors [56-L.7, 56-L.8].

56-L.3 Recent Progress

56-L.3.1 Alloy selection based on predictive models

Using the model for athermal yield stress developed by Coury et al. [56-L.4], several initial off-equimolar ternary candidate compositions with high athermal yield stress have been identified by Ben Ellyson. Thermo-Calc CALPHAD simulations were run to calculate phase equilibria with temperature for these and the corresponding equimolar compositions to determine which compositions would likely exhibit a single-phase, BCC structure across the temperature range of interest (~900-1300 °C). Using the results from the athermal solid solution strengthening model and the CALPHAD simulations, four ternary alloys with off-equimolar compositions have been selected for experimental testing. These alloys include $Mo_{0.44}Nb_{0.3}V_{0.26}$, $Nb_{0.27}V_{0.27}W_{0.46}$, $Ta_{0.22}Ti_{0.3}W_{0.47}$, and $Ta_{0.24}V_{0.33}W_{0.43}$, and their corresponding equimolar compositions. All eight compositions have predicted single-phase BCC structures with athermal yield stress above 500 MPa. Cr-containing alloys are predicted to have higher athermal yield stresses, but CALPHAD simulations predict significant Laves phase formation and limited BCC phase stability, as demonstrated in **Figure 56-L.1b**, in comparison to non-Cr-containing ternaries, which often predict single-phase BCC structures across wide temperature ranges (**Figure 56-L.1a).**

56-L.3.2 Identifying limitations in current models

Gaps in the literature data available for ternaries NbTaTi and NbTiZr across composition space between the temperatures of ~1000-1700 °C have also been identified. These gaps limit the efficacy of CALPHAD simulations for predicting phase equilibria across composition space within the identified temperature range. Further investigation into what compositions and temperatures can be found in literature will give insight into where models will be limited and will guide experiments to generate data that can be used to fill the identified gaps.

56-L.4 Plans for Next Reporting Period

Predictive models have identified several alloys for further investigation. For the next reporting period, the majority of work will focus on:

- Further literature review
- Producing equilibrium phase data for NbTaTi and NbTiZr at various compositions at temperatures ranging from 900-1300 °C
    - Identifying compositions of interest based on gaps in literature data
    - Producing buttons of selected compositions via arc melting
    - Heat treatment to reach equilibrium phases and characterization of equilibrium structures at various temperatures and compositions
- Preliminary characterization and thermomechanical processing of selected ternary and quaternary compositions
    - Refining selection of ternary and quaternary compositions based on solid solution strengthening and CALPHAD phase equilibria models
    - Producing buttons of selected compositions via arc melting
    - Initial characterization and thermomechanical processing of resultant samples

56-L.5 References

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[56-L.8] R.W. Buckman, R.C. Goodspeed, Precipitation Strengthened Tantalum Base Alloy, 1971.

56-L.6 Figures and Tables

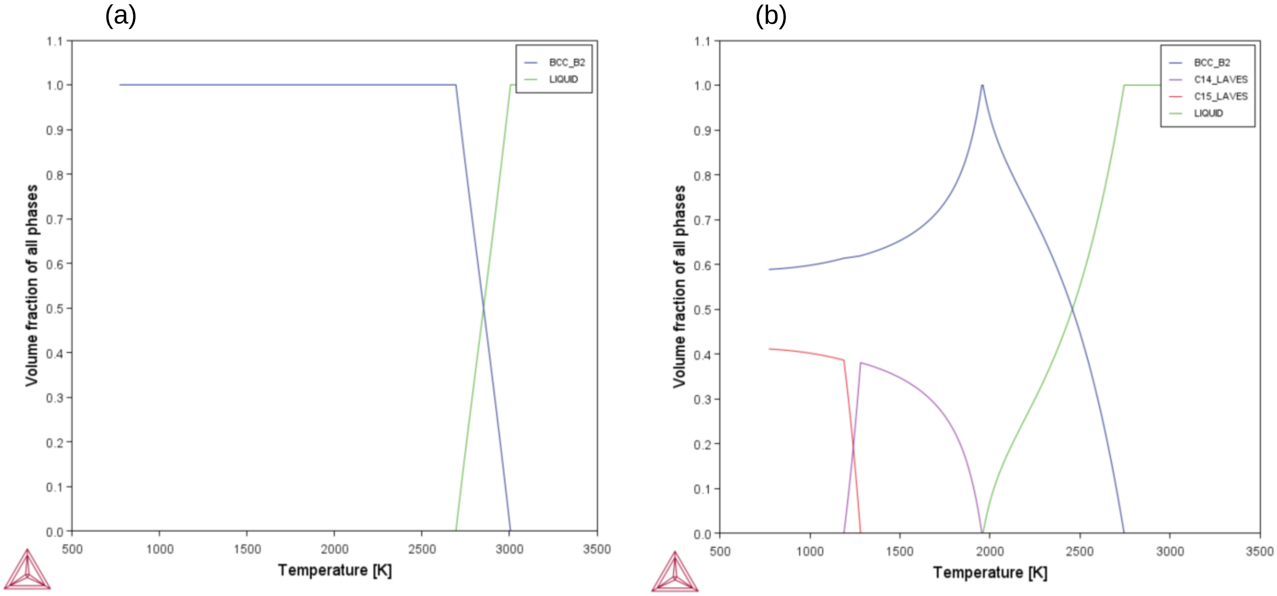

Figure 56-L.1: Phase equilibria with temperature curves for (a) $Nb_{0.27}V_{0.27}W_{0.46}$ and (b) $Cr_{0.33}Nb_{0.36}W_{0.31}$ found using Thermo-Calc CALPHAD methodology. Both alloys are predicted to have athermal yield stress greater than 500 MPa using the TC-EARS methodology. $Nb_{0.27}V_{0.27}W_{0.46}$ (a) has the highest predicted athermal yield stress, 683 MPa, for ternaries with a stable single-phase BCC region. $Cr_{0.33}Nb_{0.36}W_{0.31}$ (b) and other Cr-containing ternaries had higher predicted athermal yield stress, but are predicted to have significant Laves phase formation and little to no stable single-phase BCC region.