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I/UCRC Executive Summary - Project Synopsis	**Date**: April 2022
Center/Site: CANFSA/Colorado School of Mines	
Tracking No.:43: Thermodynamics of refractory Alloys	**E-mail :** rppuerling@mines.edu
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Center/Site Director: CANFSA/M. Kaufman/P. Collins/A. Clarke	**Type: (Continuing)**
Project Leader: Robert Puerling	**Proposed Budget**:

Project Description: Refractory multi-principle element alloys (RMPEAs) are a possible solution to the growing need for advanced structural metallic alloys capable of ultrahigh temperature performance in extreme conditions. To increase the speed at which RMPEAs can be developed, CALPHAD predictive capabilities need to be improved by filling holes in the databases, where refractory alloys are concerned.

Experimental plan: Through literature review and the assessment of CALPHAD databases for holes in fundamental thermodynamic data for refractory alloys, the ideal binary or ternary alloy(s) for experimentation will be identified. Thermo-Calc's Diffusion module (DICTRA) will be used to guide the development of the heat treatment plan. Diffusion couples will be made of pure Ta with different binary compositions of MoNb, which will then be heat treated. Heat treated samples' microstructure characteristics and phase stability will be analyzed, and resulting data will be input to CALPHAD databases.

Related work elsewhere: The majority of previous work has been focused on developing RMPEAs. This development is often guided by CALPHAD predictions.

How this project is different: Few recent studies have focused solely on improving the predictive capabilities of CALPHAD. This fundamental research will ultimately lead to the improved development of RMPEAs.

Milestones for the current proposed year: Completion of microstructure and phase stability investigation, implementation of results into CALPHAD databases, write and defend thesis.

Deliverables for the current proposed year: Journal publication comparing published solidification and homogenization data for RMPEAs MoNbTaTi and NbTaTiW to Thermo-Calc predictions. Journal publication discussing MoNbTa phase stability and microstructure and their implementation into CALPHAD databases.

How the project may be transformative and/or benefit society: An in-depth understanding of MoNbTa will be developed, with respect to phase stability and microstructure characteristics at temperatures from 1500 to 2000 $^{\circ}$C. The experimental methods employed can be further used to investigate other refractory ternaries, of which little is known. The results from this project will improve our predictive capabilities for the discovery and design of ultrahigh temperature RMPEAs for performance in extreme environments.

Research areas of expertise needed for project success: Access to: CALPHAD databases for the development of a heat treatment plan; high temperature (up to 2000 $^{\circ}$C) vacuum furnace(s) for long heat treatments; light optical microscopy, x-ray diffraction, and scanning electron microscopy for microstructure characterization and phase stability analysis. Hardness measurements may also be performed.

Potential Member Company Benefits: Improved CALPHAD databases for refractory metals will assist in CALPHAD-guided RMPEA development. Development of RMPEAs will result in new metallic alloys for use in ultrahigh temperature environments.

Progress to Date: Selection of refractory ternary alloy for experimentation (MoNbTa), as well as the high throughput diffusion couple method to be utilized to generate experimental results. Assessment of the Scheil module for predicting solidification microsegregation in refractory alloys and DICTRA's capabilities to guide the development of a heat treatment plan. Development and implementation of heat treatment plan, 1700°C for 500 hours. Initial investigations into heat treated MoNbTa phase stability and microstructure.

Estimated Start Date: Spring 2020	**Estimated Knowledge Transfer Date**: Summer 2022

The Executive Summary is used by corporate stakeholders in evaluating the value of their leveraged investment in the center and its projects. It also enables stakeholders to discuss and decide on the projects that provide value to their respective organizations. **Ideally, the tool is completed and shared in advance of IAB meetings to help enable rational decision making.**