Karlsruhe Institute of Technology

CALPHAD 2025

52nd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry

Phase formation in Ta-Mo-Cr-Ti-Al refractory high entropy alloys: CALPHAD-aided predictions and experimental study

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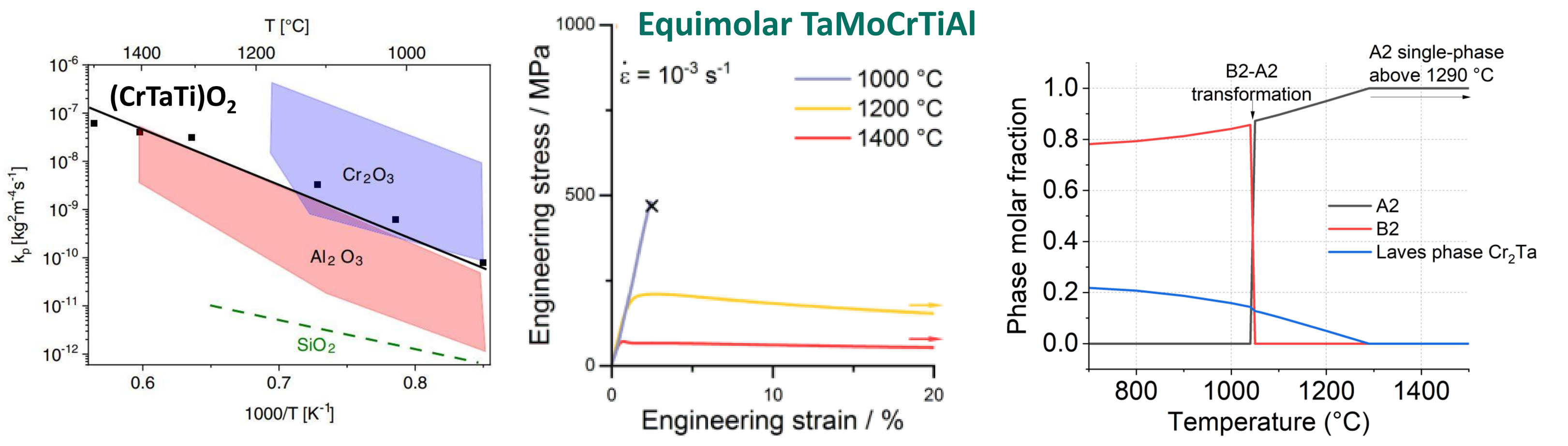
Motivation and Overview

- State of the art: Ni-based superalloys, the most used material in airplane turbines (solidus temperature T_s≈1450°C), maximal operating temperature ~ 1150°C.
- Ta-Mo-Cr-Ti-Al refractory high entropy alloys (RHEA): (1) solidus temperature T_s≈1900°C, (2) high oxidation resistance (provided by CrTa-based oxide), (3) acceptable density and high temperature strength, (4) low room temperature ductility [1-3].
- Ta-Mo-Cr-Ti-Al alloys with a dominant disordered body centered cubic (BCC) A2 crystal structure are considered favorable for enhancing room temperature ductility



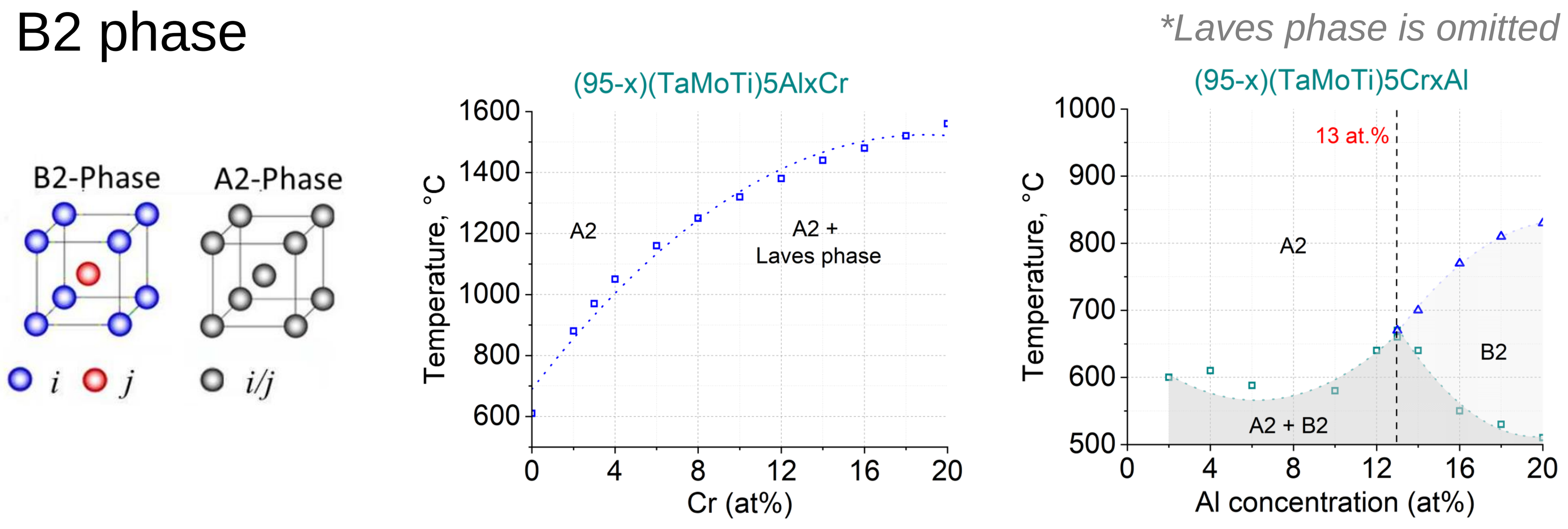
CALPHAD-aided prediction of phase formation in Ta-Mo-Cr-Ti-Al alloys

- Equilibrium calculations using CALPHAD (CALculation of PHAse Diagrams) method in alloy design with in-house thermodynamic database

Target phase constitution

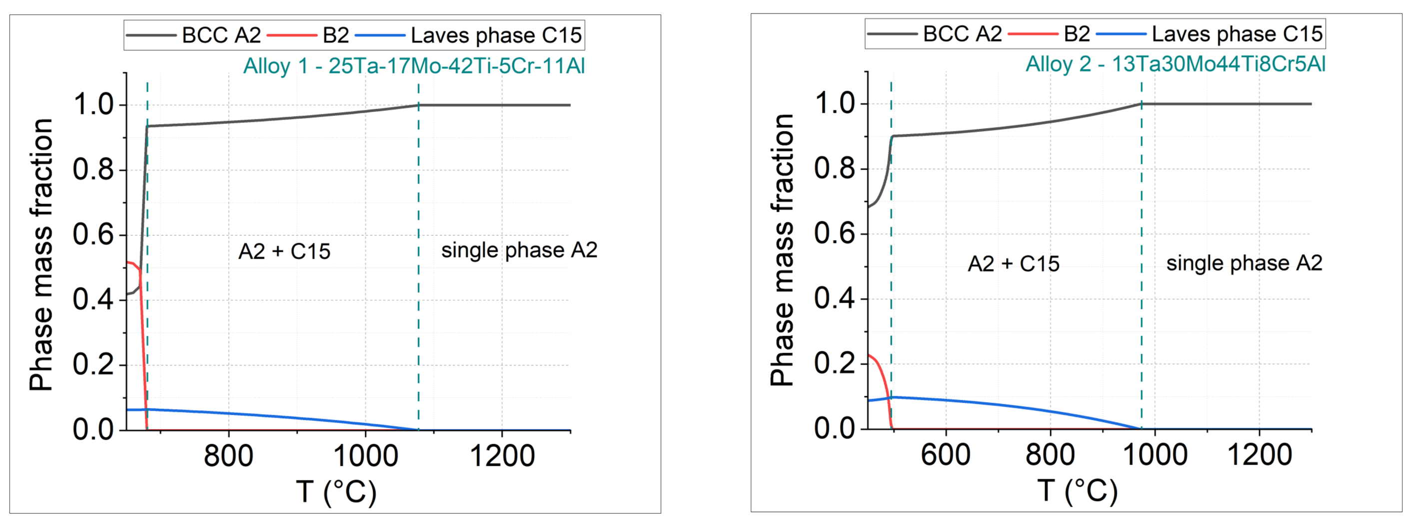
- Dominant disordered BCC A2 in the temperature range of 700-1000°C
- Low Cr concentration to inhibit the formation of Laves phases (Cr_2Ta)
- Al content below 13 at.% to prevent formation of the ordered B2 phase

*Laves phase is omitted



Identified alloy compositions

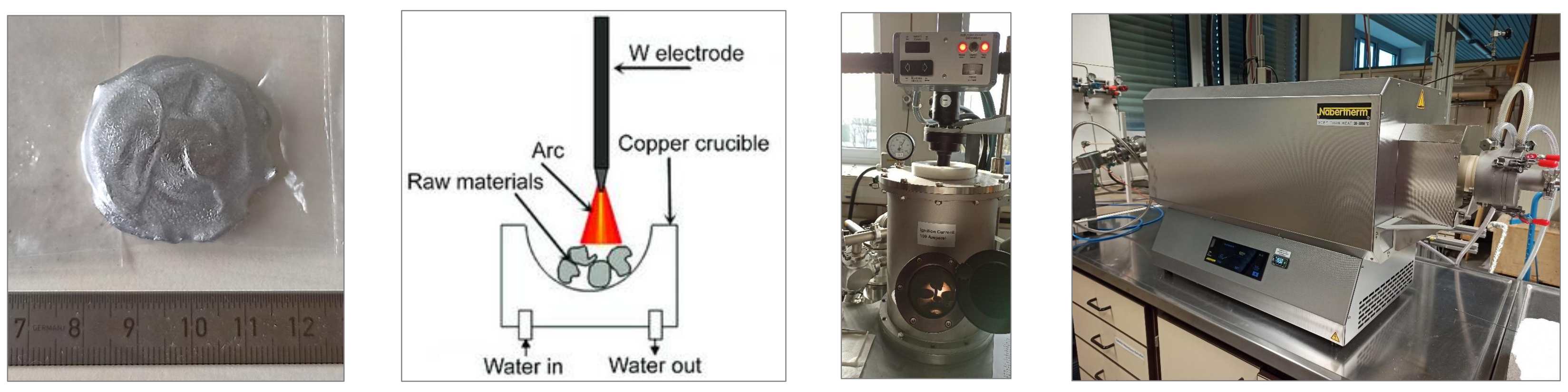
- Two alloys with targeted phase constitution and reduced density are predicted: 25Ta17Mo42Ti5Cr11Al (Alloy 1) and 13Ta30Mo44Ti8Cr5Al (Alloy 2) (at.%).



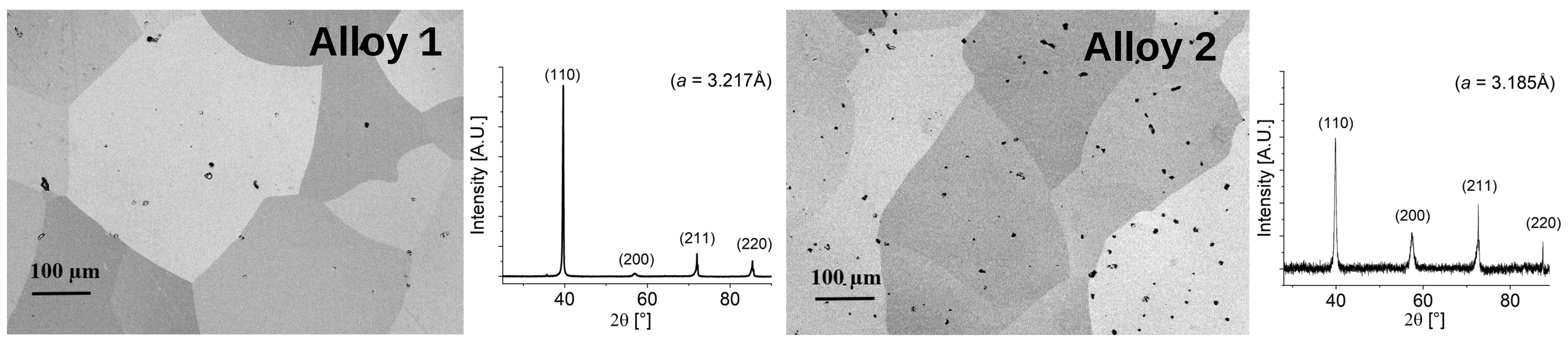
$\rho_{theor} = 8.50\ \frac{g}{cm^3}$ $\rho_{theor} = 7.90\ \frac{g}{cm^3}$

Manufacturing and Microstructure

- Manufacturing: arc melting, homogenization at 1500°C, 20 h in Ar and cooling with the rate 100 K/h



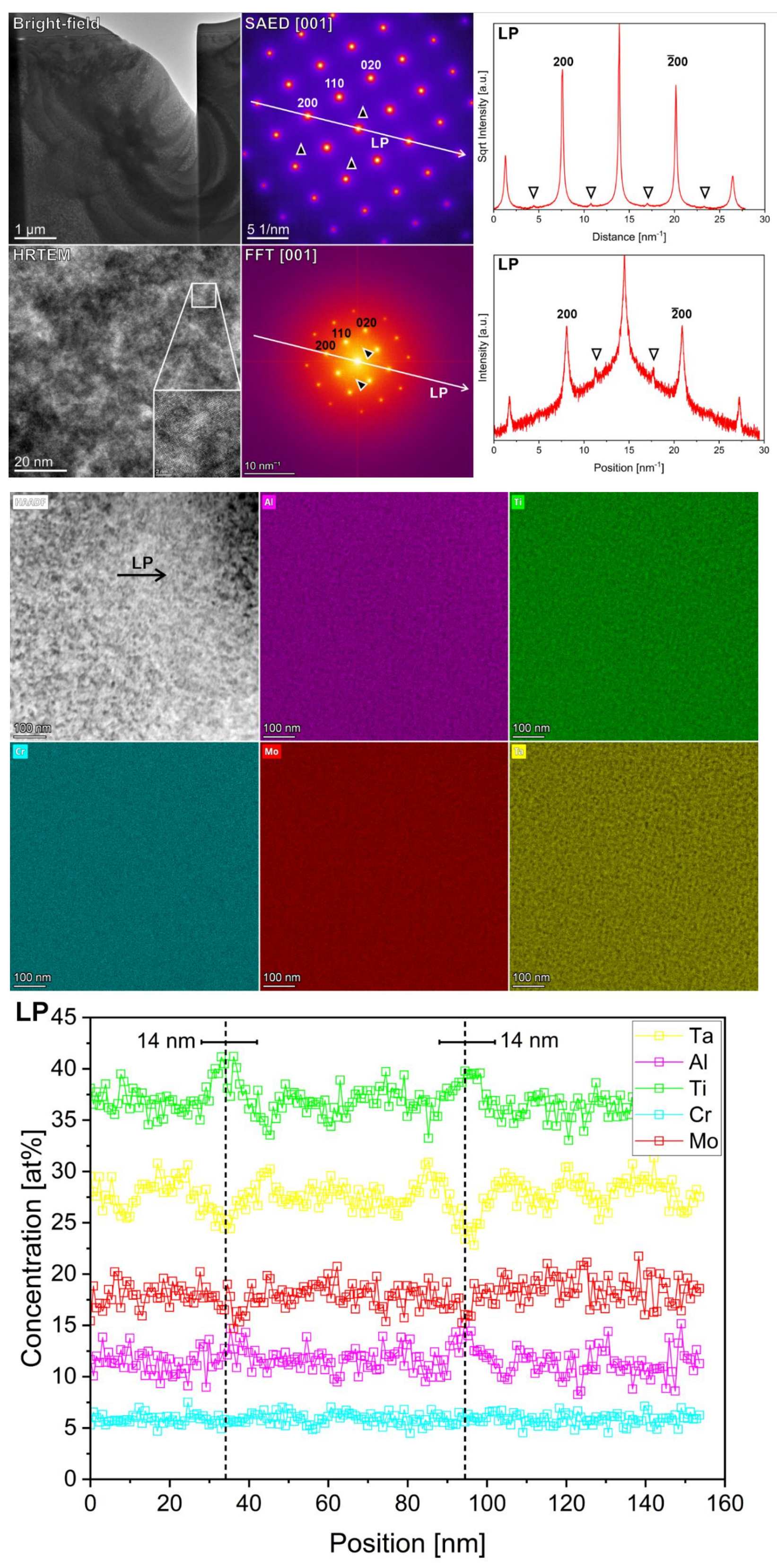
- Backscatter electron imaging: single-phase microstructure, coarse grains
- X-ray diffraction: single-phase BCC crystal structure



High-resolution transmission electron microscopy (SAED, FFT, STEM-EDX)

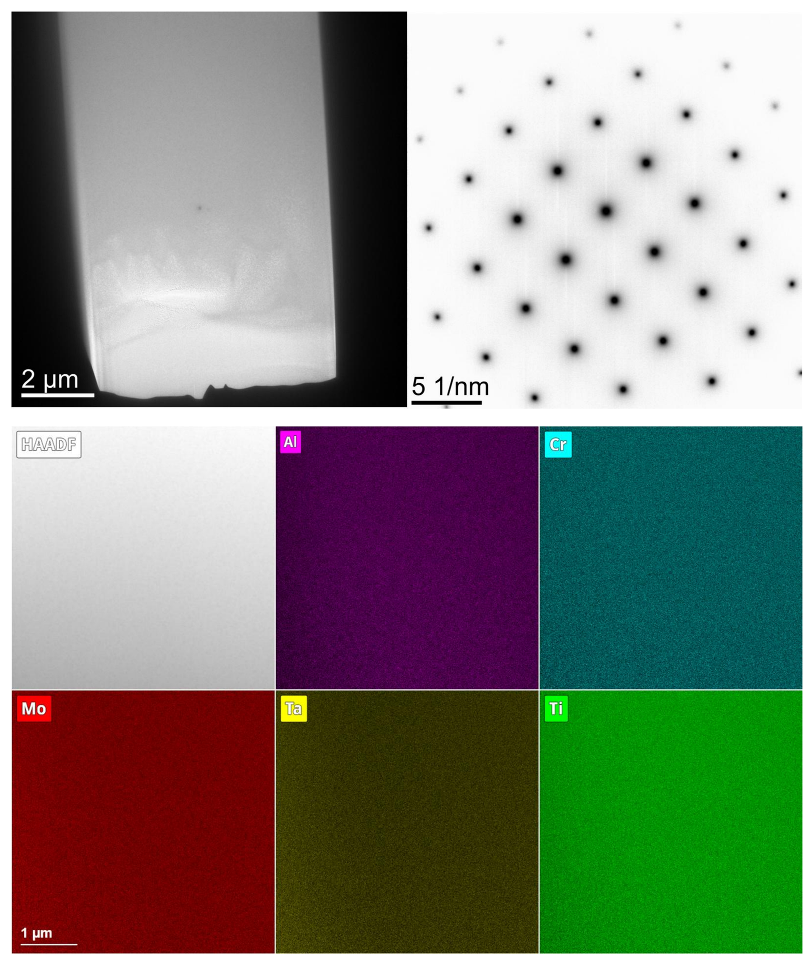
Alloy 1

- Strong A2 / weak B2 reflections
- Dominating A2 with nano-sized B2 domains
- 14 nm sized areas enriched in Ti and Al and depleted in Ta



Alloy 2

- Single-phase disordered A2 microstructure
- Homogeneous distribution of all elements



Conclusion

- CALPHAD-guided design of Ta-Mo-Cr-Ti-Al alloys with enhanced room temperature ductility and reduced density is performed
- Ultra-high resolution electron microscopy and spectroscopy required to distinguish between A2 and B2 phases

[1] S. Schellert et al. *Corrosion Science*, 2023, 211, 110885.

[2] S. Laube et al. *Acta Materialia*, 2021, 218, 117217.

[3] B. Gorr et al. *Advanced Engineering Materials*, 2021, 23(5), 2001047.

[1] [2] [3]

Bundesministerium für Wirtschaft und Energie

DLR Deutsches Zentrum für Luft- und Raumfahrt German Aerospace Center

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