Chair of Materials Engineering of Additive Manufacturing
TUM School of Engineering and Design
Technical University of Munich

Master Thesis / Semester Thesis

# Computational material design for improved mechanical performance in Ni-based alloys using the CalPhaD methodology

**Motivation**

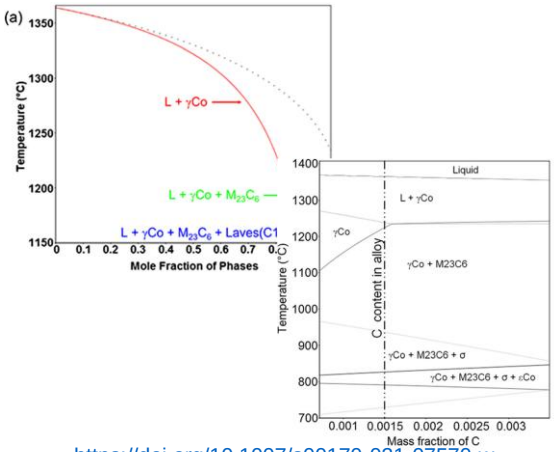
Ni-based alloys are widely used in high-temperature applications such as aerospace and power generation, but their susceptibility to cracking limits performance and service life. Computational methods such as the CALculation of PHAse Diagrams (CalPhaD) approach provide a powerful tool for designing alloys with improved crack resistance by predicting phase stability, precipitation behavior, and microstructural evolution. This research will use thermodynamic and kinetic simulations to optimize alloy compositions and processing conditions to reduce the risk of cracking and improve material performance.

**Objective**

This thesis aims to use the CalPhaD methodology to design Ni-based alloys with enhanced cracking resistance by predicting and optimizing phase formation, precipitation kinetics, and microstructure evolution. The research will focus on computational modeling to establish composition-property relationships, guiding the development of alloys with improved mechanical performance and durability.

**Tasks**

- Literature review.
- Computational simulations.
- Data analysis and interpretations.
- Validation and case studies.
- Report writing and documentation.

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**Your profile**

- Prior experience with computational materials science is desirable
- Familiarity with CalPhaD-based software (e.g., Thermo-Calc) or thermodynamic modeling is an advantage
- Ability to work independently and conscientiously.
- Good proficiency in English (written and spoken).

**Contact**

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