Bachelor / Master - Thesis Microstructure-property correlation via

object oriented Finite Element analysis

Helmholtz-Zentrum Hereon, Institute of Materials Mechanics, Solid State Materials Processing (WMP)



Introduction

The properties of materials depends on the amount and distribution of phases in the microstructure. The characteristics of the individual phases may be known from single-phase calculations. However, in real systems, the properties vary significantly with change in size and shape of the second-phase particles inside the matrix. Effect of externally applied stress and the deformation induced during mechanical processing also affects the microstructure and subsequently the properties. In fact, the properties may not isotropic in most cases. The feature dependence forms the motivation to investigate such microstructure-property correlation which is an integral part of the multi-scale modelling approach.



The main objective of this work is to compute the macroscopic properties of microstructures using object oriented finite element analysis. The method involves adaptive meshing for improving performance as shown in Figure 1. It is possible to predict the net elastic moduli, stress and strain distributions etc. by relevant FEM calculations similar to Figure 2. The computed values serve as guide to design microstructures with desired properties. Several already obtained microstructures from mesoscale models or from experiments usually serve as inputs to the study. The specific alloys that are of interest here are the Al-rich binary and ternary systems.

The place of employment would be Helmholtz-Zentrum Hereon

Input microstructure Mesh generation Mesh adaption

Figure 1: Overview of the different steps involved during macroscopic property calculation of a reference input microstructure.



Figure 2: Sample results showing stress and strain distributions inside the microstructure computed using object oriented finite element

Tasks

- Comprehensive literature review on existing Finite Element modules for macroscopic property calculation.
- Design of input modules and calculation of properties.
- Compilation of post-processing tools for microstructure data analysis.
- Presentation of results and documentation of the work (in English).

Expectations

- Decent knowledge of phase transformations, diffusion, elasticity, and plasticity in general.
- Fundamental understanding of Finite Element Method.
- Proficiency in object-oriented programming (preferably C++, python).
- Readiness to learn new software, skills and punctually deliver as per the project requirement.

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