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Integrated Computational Materials Engineering - ICME

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ABSTRACT

The production of increasingly complex and valuable goods requires highly advanced, knowledge-based, tailored materials and components. To meet the ambitious objective of life-cycle modelling of products is an integrative description of the component history, starting e.g. from a homogeneous, isotropic melt; continuing via subsequent process steps, and ending ideally in the description of failure onset under operational load. The realisation of such a modelling scenario at different scales is one of the key objectives of ICME. Its focus is on engineering the component properties as a function of *local material properties* at the micro- and nano-scale. These properties themselves have experienced an evolution and depend on the entire manufacturing process history as well on the design of the component and on the alloy composition. Another key objective of ICME is to combine high-throughput or high accuracy material characterization of materials with novel multi-scale simulation methods to predict more accurately material properties. Their skilful combination will lead to significant improvements in e.g. prediction of phase stability in multi-component materials, accelerates materials development and unifies design and manufacturing.

The aim of this mini-symposium is to present novel developments and discuss recent advances on ICME related topics, including following aspects:

- Multi-scale modelling of different manufacturing process steps of a component;

- Standardization of data transfer between models acting at different scale or manufacturing steps;
- Spatial representation of complex microstructures: generation and discretization of realistic RVE of these heterogeneous microstructures;
- New computational mechanics tools based on materials physics in order to predict more accurately material properties (e. g. efficient solvers for microstructure-based simulation, like Lippman-Schwinger (FFT, SLS,…) or model reduction methods (POD, PGD), …) ;
- Microstructure-based materials processing models combined with high-accuracy material characterization methods (EBSD, TEM, …);
- Material design based on numerical concurrent methods combining different scale algorithms;
- Inverse problems in material design: tailor microstructure to optimize material properties;
- Materials: alloys, composites, functionally graded materials, concrete, …