EUROMAT 2019 / Area D

SYMPOSIUM: D4

Title: Integrated computational materials engineering and design

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Abstract

Integrated Computational Materials Engineering, ICME, and materials design can decrease materials development time drastically. In order to succeed, the gap between *ab initio* and empiric or semi-empiric methods has to be bridged and thermodynamic and kinetic properties of relevant alloys may be obtained by combining *ab initio*, phenomenological methods and experimental results. In line with this development, this symposium is dedicated to multiscale materials modelling focusing on the structure and properties of materials and the relation between them. One area of interest is modelling of phase transformations including the effect of deformation and its effect on the materials properties. This includes the stability of the bulk as well as grain boundaries, nucleation, growth, point-defects, dislocations and their interactions. It is thus necessary to understand and model phenomena covering length scales from pico-meters (e.g. atoms) to meters (e.g. a sailing boat).

We invite discussions, reports of implementation and illustrations of applications of multiscale materials modelling, directly or indirectly, including at least two scale levels. The section does not restrict the kind of material (organic, inorganic) or application (medical, energy, construction, etc)

Targeted Topics

- Multi-scale modelling
- Atomistic modelling
- Molecular dynamics
- Phase-field modelling
- Thermodynamic modelling
- Kinetic modelling
- Dislocation-based modelling
- Phenomenological modelling
- Continuum modelling