Microstructure driven design of materials

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Recently, new experimental and in-situ diagnostic techniques, coupled with advanced microstructure characterization and modeling techniques, are starting to allow for detailed study of complex properties and processed (elastic and plastic deformation, impact, fatigue, fluid flow and mass transport, catalysis, etc.) and what is crucial their linkage to microstructure. Moreover, these experimental advancements have been accompanied by radical progress in numerical capabilities enabled by modern computers.

The weight of large-scale computations has given an amazing predictive capability to the field and an ability to incorporate large data sets collected by modern experiments into mathematical models. Present material model development - in general, is largely dependent on continuum scale phenomena and ignores the rich multiscale physical and chemical phenomena that are responsible for the macro-scale response of materials. The substantial complexity of these phenomena, which occur through the specific microstructure and its evolution in response to various loading conditions, presents significant challenges to theoretical model development in computational modeling, therefore it is a field for Integrated Computational Material Engineering (ICME).

This minisymposium aims at design of materials properties and processes controlled by their microstructure. The design involves numerical modeling and experimental techniques towards understanding of microstructure-property relationships. The scope of minisyposium encompasses structural and functional aspects of various groups of materials such as: polycrystalline, cellular, porous and composites.

Thus, participation in this mini-symposium will help to understand and control properties of mentioned group of materials with fundamental and practical interest across various scales by developing and using new advancements in computational modeling.

The aim of this mini-symposium is to address through scale challenges in development of numerical methods dedicated to microstructure driven materials design. Researchers addressing following topics are invited to submit their contribution:

- Modeling mechanics of polycrystalline materials.

- Modeling mechanics of lightweight materials and composites.

- Modeling of functional properties of materials.

- Modeling of materials processes.

- Computational methods in materials modeling, such as Homogenization Method (HM), Monte Carlo (MC) method, Cellular Automata (CA) method, Molecular Dynamics (MD), Dislocation Dynamics (DD), etc. This also involves multiscale approaches.