Special Issue

Computational Design of Complex Structural Alloys

Message from the Guest Editors

Modelling tools have recently developed into a such stage where they are of a valuable help to steer the development and optimisation of novel structurally complex alloys. Still, in order to obtain picture which is of practical relevance at experimental length-scales, information from several levels of modelling insight must be combined. Quantum mechanical calculation provide description of the inter-atomic interactions on the very fundamental level; atomistic methods are suitable for studying extended defects (e.g., grain boundaries, dislocations, cracks etc.) and their mutual interactions; finally, mesoscopic continuum thermodynamics methods are suitable for describing the microstructural evolution. The intention of this special issue is to attract contributions combining ab initio, atomistic (molecular statics/dynamics or Monte Carlo) and thermodynamic (phase field and CALPHAD) modelling approaches with experimental works. The contribution should show the state-of-the-art in predicting composition and microstructure and thus to not only provide explanation for various phenomena occurring in multi-phase structural alloys, but also to guide their further improvement.

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Message from the Editor-in-Chief

Materials (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

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