Special Issue

Applications of First-Principles or Reliable Force Field Methods to Determine Microstructures or Phases of Metals and Alloys

Message from the Guest Editors

The number of possible phases of alloys is exponentially enormous. Therefore it would be quite inefficient to attempt to investigate very different microstructures based only on experimental approaches. The use of computer simulation techniques such as phase field (PF) models, large-scale molecular dynamics (MD), and Monte Carlo (MC) simulations as well as quantum mechanical DFT or other first-principles calculations may greatly assist the experimental investigations.The reliability of MD and MC simulations strongly depends on the force field to be used. In these situations, there is a strong demand for the development and application of reliable multiscale or nanoscale simulation methods based on first principles. One of the idea would be to combine PF modeling or some other modeling techniques, including MD and MC, with a first-principles method or a highly reliable force field. Our aim is to cover the recent progress and new developments regarding all aspects of reliable multiscale or nanoscale simulations in investigating the microstructures and phases of metals and alloys.

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Metallic materials play a vital role in the economic life of modern societies; contributions are sought on fresh developments that enhance our understanding of the fundamental aspects related to the relationships between processing, properties and microstructure – disciplines in the metallurgical field ranging from processing, mechanical behavior, phase transitions and microstructural evolution, nanostructures, as well as unique metallic properties – inspire general and scholarly interest among the scientific community.

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