Special Issue

Multiscale Modeling

Message from the Guest Editors

The physical and mechanical properties of materials are largely determined by their microstructure, as well as defect and impurity concentrations. To understand and control these changes during aging, loading, irradiation, and annealing require different simulation techniques to link the complex physics involved at different time and length scales. The different scale simulation approaches, which together constitute multiscale modeling, extend from density-functional theory to rate equations and finite-element modeling. Recent advances in simulation techniques and in the understanding of defect interactions have improved the reliability of multiscale modeling and extended its use in simulating various dynamic processes in solid materials. In this Special Issue, recent advances in multiscale modeling techniques, including relevant fundamental defect interactions at different time and length scales, are highlighted and discussed.

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