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MULTISCALE MODELING AND EXPERIMENT

Synergies between computational modeling and experimental characterization of materials across length scales

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Materials Science is highly interdisciplinary; greater insight into structure–properties relationships requires the development of multiscale/multiphysics models and comparably advanced experimental design, instruments, and analysis. Such challenges and expanding research scope motivate synergies between experimental and the computational communities. Outcomes of this emerging field within the Materials Science community open up new frontiers and research directions at the crossroads of traditional computational Materials Science, experimental Materials Science, and Integrated Computational Mechanics. Such cooperative interactions find many applications in the development, the characterization, and the design of complex material systems.

The manuscripts for this special section included in this issue of the Journal of Materials Science highlight examples of recent advances in coupled computational/experimental approaches in predicting various physical phenomena and mechanisms in materials. The manuscripts can be grouped into several topical areas that include: (i) Materials Science at the atomistic scale; (ii) The development of approaches for heterogeneous microstructures; and (iii) 3-D microstructure analysis, including microstructure evolution and mechanical behavior at the microscale.

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In "Review of the Synergies Between Computational Modeling and Experimental Characterization of Materials Across Length Scales," we provide a broad and comprehensive overview of recent trends where predictive modeling capabilities are developed in conjunction with experiments and advanced characterization. This review article highlights recent synergies at various scales both from an experimental perspective and from a modeling perspective, discussing the roles of experiments in multiscale models and vice versa. This review article ends with a discussion on some problems and gaps that have to be addressed in order for this coupled approach to impact research and development in the broad scope of structure–property relations successfully in the future.

Yamakov et al.'s "Multiscale Modeling of Sensory Properties of Co–Ni–Al Shape Memory Particles Embedded in an Al Metal Matrix" features an atomistic-to-continuum multiscale model to study the efficacy and variability in the sensory particle transformation to detect damage processes in novel ferromagnetic shape memory alloys. This manuscript exemplifies recent efforts within the modeling community to develop new algorithms and methodologies to not only bridge length scales within heterogeneous microstructures but also to account for the multiphysics dimension associated with such complex materials systems.

In "Experimental and computational studies on the role of surface functional groups in the mechanical behavior of interfaces between single-walled carbon nanotubes (CNTs) and metals", Hartmann et al. investigate the structure–property correlation of single-walled CNTs embedded in a noble metal (Pd or Au) through the combination of an experimental and computational approach. The experimental component consists of nanoscale pull-out tests with in situ scanning electron microscope experiments, while

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the computational component relies on molecular dynamics simulations to predict force-displacement during pull-out. A particular emphasis is put on the role of surface functional groups covalently linked to CNTs. This manuscript provides a very good example of how experimental testing combined with computational tools can be used as an efficient investigative tool to study structure–property relations in novel material systems.

In "Development of an in situ method for measuring elastic and total strain fields at the grain scale with an estimation of accuracy," Chow et al. conduct in situ experimental measurements based on Digital Image Correlation and X-ray diffraction to identify parameters used in grain-level crystal plasticity models. This work illustrates how recent experimental advances in local field measurements have been impactful within the modeling community.

In "Bridging atomistic simulations and experiments via virtual diffraction: Understanding homophase grain boundary and heterophase interface structures," Coleman et al. describe advances in the use of virtual diffraction within an atomistic framework as a method to study the geometry and structure of grain boundaries and interfaces. In this work, simulated diffraction patterns are used to identify the structure of Al twist grain boundaries and heterophase Al_2O_3/Al interfaces without a priori assumption of the periodic interface structure. This manuscript provides a detailed example and illustration of how well-established experimental methods such as diffraction are now being implemented directly into computational models to complement and support the interpretation of experimental results.

Finally, in "Phase field modeling for grain growth in porous solids," Ahmed et al. present a detailed investigation of the grain growth process in porous solids based on 3-D simulations of a novel phase field model. This model accounts for all the possible pore-grain boundary interactions and microstructural features affecting the overall growth kinetics to investigate the effect of porosity on the kinetics of grain growth in CeO_2 in 3-D. Model results were found to agree well with published experimental data. This manuscript thus provides an example of the characterization and modeling of in-volume microstructural behavior.

In summary, this short collection of manuscripts is intended to provide the researchers and engineers in the Materials Science community with recent successes of predicting various physical phenomena and mechanisms in materials systems enabled by the collaboration between experimentalists and modelers. It is hoped that this special section will not only provide insights into how computational materials science can be exploited as discovery tools for materials engineering rather than "simply" supporting experimental work but also inspire readers of the Journal of Materials Science to further advance this emerging field.

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