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A DESCRIPTOR-BASED DESIGN METHODOLOGY AND MATERIALS INFORMATICS FOR DEVELOPING HETEROGENEOUS MICROSTRUCTURAL MATERIALS SYSTEM

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In designing a microstructural materials system, there are several key questions associated with design representation, design evaluation, and design synthesis: how to quantitatively represent the design space of a heterogeneous microstructure system using a small set of design variables, how to efficiently reconstruct statistically equivalent microstructures for design evaluation, and how to quickly search for the optimal microstructure design to achieve the desired material properties. We propose a new descriptor-based methodology for designing microstructural materials systems. It is proposed to use statistical learning to identify a small set of microstructure descriptors to represent material morphology features quantitatively. The descriptor set cover critical microstructure features at different levels, including composition, dispersion status, and phase geometry. The descriptor-based representation allows efficient stochastic reconstructions of microstructures in both 2D and 3D spaces for Finite Element Analysis (FEA) to predict material properties and the use of probabilistic optimization approach to search the optimal microstructure design. To improve the search efficiency, we integrate state-of-the-art computational design methods such as Design of Experiment (DOE), metamodeling, statistical sensitivity analysis, and multi-objective optimization, into one design optimization framework to automate the microstructure design process. The proposed methodology is demonstrated using the design of a polymer nanocomposites system. A material informatics system entitled Nano-Mine is established to mine he existing data in literature and predict the relationships between process to microstructure to properties in designing new microstructural materials systems.

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