Communications, Networking, Signal & Image Processing

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"Novel and Enhanced Structure-Property-Processing Relationships with Microstructure Informatics"

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Abstract

Advances in computational materials science and novel characterization techniques have allowed scientists to probe deeply into a diverse range of materials phenomena. These activities are producing enormous amounts of information regarding the roles of various hierarchical material features in the overall performance characteristics displayed by the material. This data deluge poses a significant challenge in effectively utilizing the microstructure information to develop structure-property-processing connections. Microstructure Informatics (μInformatics) is an emerging data-driven paradigm that leverages the rich 2-D and 3-D spatiotemporal physical data being generated across the materials science community. μInformatics is built upon a stochastic framework that utilizes spatial distribution functions (e.g. n-point correlation function, chord length distributions, interfacial shape distributions) to develop rich bi-directional structure-property-processing relationships and next generation materials taxonomies. The spatial distributions transform raw physical materials data into forms that are amenable to a variety of pre-existing digital signal processing techniques (e.g Filter Design, Reconstruction Algorithms) and scalable data-mining tools (e.g. Dimension Reduction, Clustering Algorithms) which are capable of exploring high dimensional data.

This work outlines the powerful utilities encompassed by μInformatics and its implications in the materials design process. A new database framework has been developed that can automatically classify and organize microstructure topologies, or by proxy their processing history, based upon rigorous statistics analysis rather than relying on ad-hoc selected metrics. It will be shown that incorporating rigorous spatial distributions enhances the accuracy and reach of instantiated homogenization relationships that predict transport properties in porous bi-layers in fuel cells. In a similar manner, μInformatics contains tools to generate scalable, parallelizable meta-models that generate top-down localization relationships vital to inverse materials design. These meta-models can accurately supplant costly simulations that generate spatially resolved structure-property (e.g. moderate contrast elastic deformation) and structure-processing (e.g. spinodal decomposition) linkages. Each of the linkages can be visualized alongside the 4-D spatiotemporal evolution of the microstructure to provide a concurrent structure-property-processing connections.

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