abstract
An accurate knowledge of the complex microstructure of a heterogeneous material is crucial for quantitative structure-property relations establishment and its performance prediction and optimization. X-ray tomography has provided a non-destructive means for microstructure characterization in both 3D and 4D (i.e., structural evolution over time). Traditional reconstruction algorithms like filtered-back-projection (FBP) method or algebraic reconstruction techniques (ART) require huge number of tomographic projections and segmentation process before conducting microstructural quantification. This can be quite time consuming and computationally intensive.

A novel procedure is presented that allows one to directly extract key structural information in forms of spatial correlation functions from limited x-ray tomography data. The key component of the procedure is the computation of a “probability map”, which provides the probability of an arbitrary point in the material system belonging to specific phase. The correlation functions of interest are then readily computed from the probability map. Using effective medium theory, accurate predictions of physical properties (e.g., elastic moduli and thermal /electrical conductivities) can be obtained.

Secondly, a stochastic optimization procedure that enables one to accurately reconstruct material microstructure from a small number of absorption contrast x-ray tomographic projections is presented. It has been shown that only a small number of projections (e.g., 20 - 40) are necessary for accurate material reconstructions via the stochastic procedure. With one step further, a stochastic reconstruction procedure with multi-modal data fusion is proposed, where both X-ray projections and correlation functions computed from 2D optical images are fused as the information input.

This multi-modal reconstruction algorithm is proved to be able to integrate the complementary data to perform an excellent optimization procedure, which indicates its high efficiency in using limited structural information.

Finally, the accuracy of the stochastic reconstruction procedure with limited X-ray projection data is validated by analyzing the microstructural degeneracy and the roughness of energy landscape associated with different number of projections. Ground-state degeneracy of a microstructure is found to decrease by increasing number of projections, which indicates higher probability of reconstructing configurations matching the target. The roughness of energy landscape can provide information about the relative complexity of the reconstruction for certain structures.