Low-dimensional models for microstructure representation: A data-driven approach

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Many areas of material science involve analyzing, linking and designing the materials internal structure (microstructure) with macro-scale properties and the processing history. The huge size of the microstructural data set precludes any straightforward analysis, particularly in the areas of stochastic analysis, process-property-structure mapping and accelerated insertion of materials. Constructing low-dimensional representations of microstructure variations would greatly simplify and accelerate such design and analysis tasks. We develop a mathematical strategy for the data-driven generation of low-dimensional models that represents the variability in polycrystal microstructures while maintaining the statistical properties that these microstructures satisfy. This strategy is based on a non-linear dimension reduction strategy to map the space of viable microstructures (M) to a low dimensional region (A). The use of Fourier and/or Radon transform allows for a straightforward method to enforce the statistical constraints. A number of examples will be presented to demonstrate these techniques and their applications.