Establishing Processing-Structure-Properties (PSP) Linkages Using Tensor Analysis

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Objectives: Develop and apply a set of novel and recently developed machine learning algorithms in the area of tensor analysis (TA) to learn low dimensional descriptors from high-dimensional microstructure data and directly establish complex processing-structure-properties (PSP) linkages targeting alloy design and performance predictions.

Technical Approach:

The proposed TA algorithms developed recently by Kamran Paynabar's research group merge the dimensionality reduction for structural feature identification and the linkage construction into a single step that improves the linkage predictions. Approaches such as the well established principal component analysis (PCA) construct the model after the dimensional reduction step is complete. A model built based on TA algorithm includes both the dimension reduction and model formation in the same regression analysis and as a result has potential for stronger prediction capability. Presently, the method needs to be evaluated on some exemplar problems to fully flesh out the workflow for using it. One example of a exemplar is linking in-service processing conditions of a high temperature alloy to how the microstructure evolves supporting remaining life predictions.

Concept Illustration:
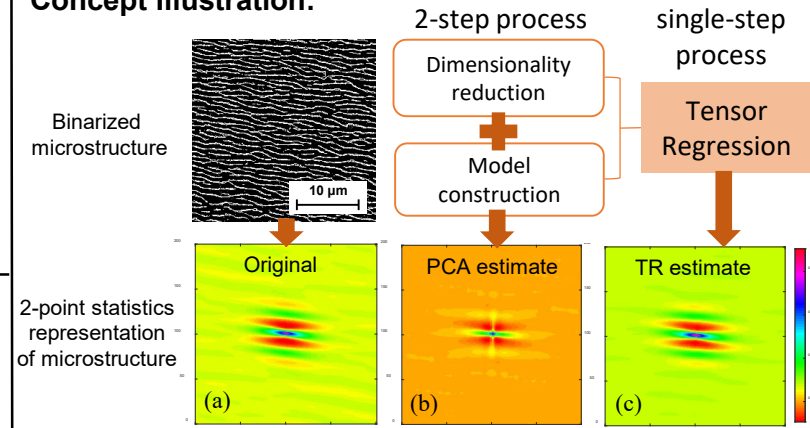
Impact: New machine learning methods applied to materials discovery, development, and deployment are needed to handle a wide range of PSP linkage problems. TA involves a set of algorithms that have not been applied to materials design, yet can potentially deal with some of the complexities in the vast variations in the type of data that needs to be linked. Materials in extreme and harsh environments are engineered to have as long of life as possible; however, their life is often finite. Accurately predicting remaining life is critical for minimizing downtime. The aim is to develop a general MATIN tool targeting developing PSP linkages using TA algorithms.`