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A Machine Learning-based Design Representation Method for Designing Heterogeneous Microstructures

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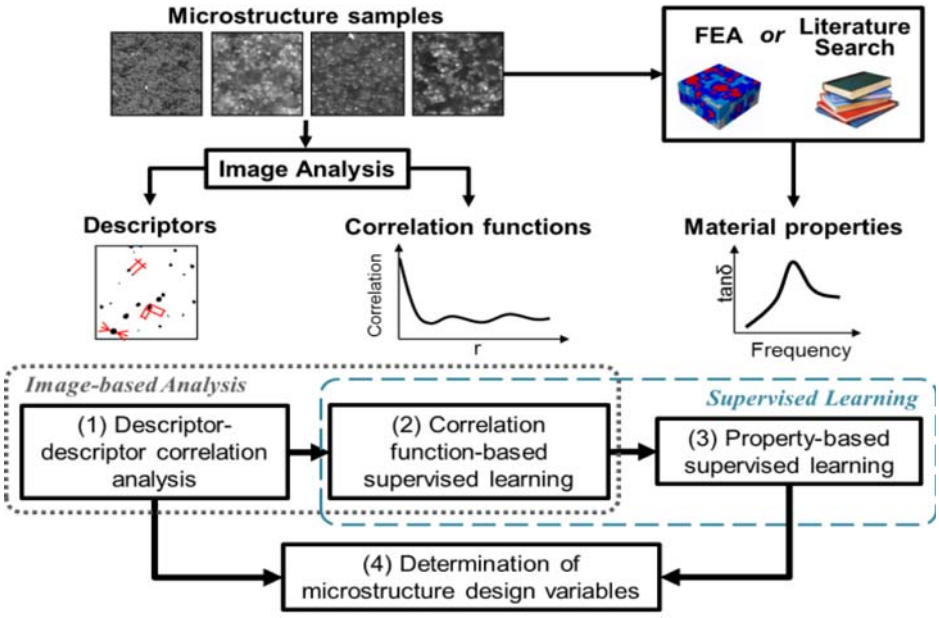

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Scientific Achievement

We developed a machine learning-based method for identifying the key microstructure descriptors from vast candidates as potential microstructural design variables. With a large number of candidate microstructure descriptors collected from literature covering a wide range of microstructural material systems, our method is able to perform 4-fold of functionalities: (1) eliminate redundant microstructure descriptors via image analyses, (2) identify key microstructure descriptors based on microstructure morphology, (3) identify key microstructure descriptors based on structure-property relationship, and (4) determine the final set of microstructure design variables. The benefits are demonstrated by an example of polymer nanocomposites optimization. We compare designs using key microstructure descriptors versus using empirically-chosen microstructure descriptors to validate the proposed method.

Significance

In designing microstructural materials systems, one of the key research questions is how to represent the microstructural design space quantitatively using a descriptor set that is sufficient yet small enough to be tractable. Existing approaches describe complex microstructures either using a small set of descriptors that lack sufficient level of details and require prior empirical identification and selection, or using generic high order microstructure functions of infinite dimensionality without explicit physical meanings. Our method solves this problem by effectively reducing the infinite dimension of the microstructure design space to a small set of descriptors without a significant information loss.

Citation Information

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