Establishment of Structure-Property Linkages Using a Bayesian Model Selection Method: Application to A Dual-Phase Metallic Composite System

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Abstract: The viability of establishing low-cost surrogate structure-property (S-P) linkages which applies a Bayesian model selection method to the Materials Knowledge System (MKS) homogenization framework is studied. The MKS framework employs the n-point correlation function, principal component analysis, and regression techniques for mapping between the structural factors and the property of a material. However, the framework chooses the factors not by their influence on the property but by their amount of inherent microstructural information. This also makes it difficult to find out which microstructural morphology affects the property. In the present work, we introduced a Bayesian model selection method to choose the important factors and interpret their implications for the property. First, the yield strengths of synthetic microstructures having various morphological characteristics are evaluated by the crystal plasticity simulation. Then, the constituent factors for microstructure-yield strength relationship are obtained from the MKS framework. Next, the microstructure-yield strength model is constructed with the influential factors chosen by the Bayesian model selection method. Lastly, the validation of the obtained model is conducted with an independent dataset and the morphological meaning of the constituent factors are analyzed by the reconstruction method based on a Monte Carlo algorithm.

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