Microstructural Materials Design via Deep Adversarial Learning Methodology

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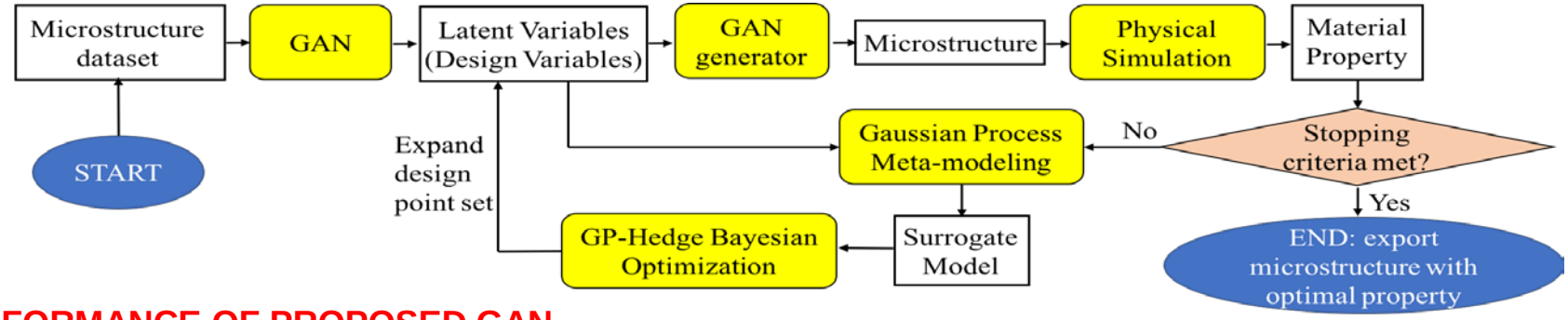
June 14, 2018

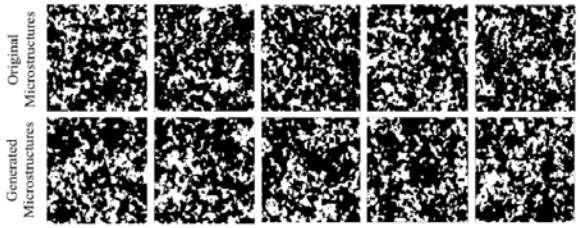
RESEARCH OBJECTIVE

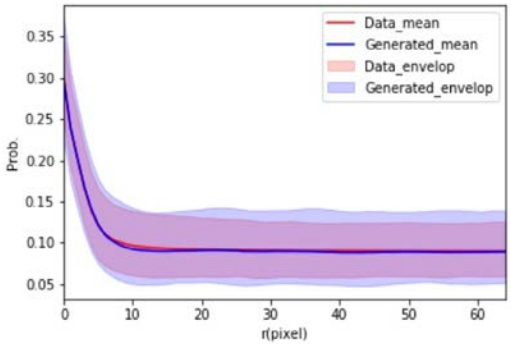
Identifying the key microstructure representations is crucial for Computational Materials Design (CMD). In this work, generative adversarial networks (GAN) are trained to learn the mapping between latent variables and microstructures. Thereafter, the low-dimensional latent variables serve as design variables, and a Bayesian optimization framework is applied to obtain microstructures with desired material property. Due to the special design of the network architecture, the proposed methodology is able to identify the latent (design) variables with desired dimensionality, as well as capturing complex material microstructural characteristics. In essence, the proposed methodology provides an end-to-end solution for microstructural design, in which GAN reduces information loss and preserves more microstructural characteristics, and the GP-Hedge optimization improves the efficiency of design exploration.



PERFORMANCE OF PROPOSED GAN

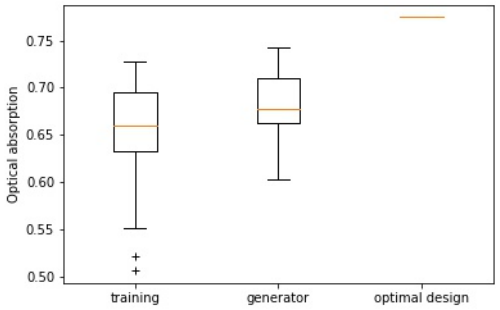
The proposed GAN can generated visually similar microstructures

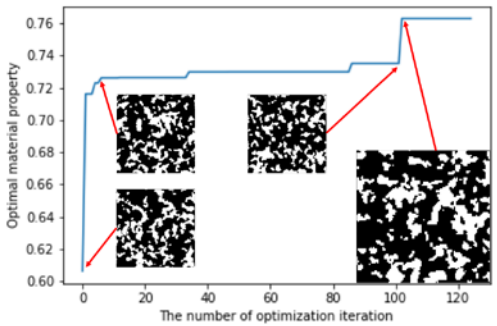




The comparison of two-point correlation shows that the statistics of generated microstructures matches that of training set.

MICROSTRUCTURE DESIGN EVALUATION





The latent variables are considered as design variable in a Bayesian optimization framework to obtain microstructures with desired material property.

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