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Deep neural network method for predicting the mechanical properties of composites

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Sang Ye, Bo Li, Qunyang Li, Hong-Ping Zhao, and Xi-Qiao Feng[a)]

AFFILIATIONS

Institute of Biomechanics and Medical Engineering, AML, Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China

[a)]Author to whom correspondence should be addressed: fengxq@tsinghua.edu.cn

ABSTRACT

Determining the macroscopic mechanical properties of composites with complex microstructures is a key issue in many of their applications. In this Letter, a machine learning-based approach is proposed to predict the effective elastic properties of composites with arbitrary shapes and distributions of inclusions. Using several data sets generated from the finite element method, a convolutional neural network method is developed to predict the effective Young's modulus and Poisson's ratio of composites directly from a window of their microstructural image. Through numerical experiments, we demonstrate that the trained network can efficiently provide an accurate mapping between the effective mechanical property and the microstructures of composites with complex structures. This study paves a way for characterizing heterogeneous materials in big data-driven material design.

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Determining the mechanical properties of composites is of great significance for their applications in a wide diversity of engineering fields.[1–3] Besides experimental characterization,[4,5] some theoretical homogenization methods have been established to estimate the macroscopically average properties of composites, e.g., self-consistent method, Mori–Tanaka's mean-field method,[6] and Chamis's micromechanical model.[7] Most of these are based on Eshelby's solution of inclusions with elliptical or other regular shapes[8] and thus hard to predict the macroscopically effective properties of composites with complex microstructures. For such complex composites, the finite element method (FEM) is normally utilized to calculate the material properties by defining a representative volume element (RVE).[3,9,10] The RVE should be sufficiently large in order to rule out the effect of RVE sizes, and, therefore, the FEM calculation is usually tedious and highly time-consuming. In addition, the RVE method is specifically sensitive to the geometric and topological features of the microstructures of composites.

The mechanical properties of a composite depend on its manufacturing process, constituent phases, and microstructures, making their determination a complex nonlinear and material-specific problem.[10] Recently, the artificial intelligence method has been extended to various problems of materials science and engineering, e.g., predicting their crystal structures and stability,[11,12] atomic and molecular properties,[13–16] complex phase transitions,[17,18] and service life.[19] In particular, the deep neural network (DNN) method has been proven to be efficient in discovering meaningful structures in data. With a sufficient amount of training data and a specific target, this method is capable of extracting the high-dimensional feature vector from the original data and learning the nonlinear mapping from the feature vector to a desired output.[11,20]

In this Letter, we propose a DNN method to predict the mechanical properties of composites with complex microstructures. Through the implementation of RVE homogenization in the FEM, we first generate multiple data sets, which contain pairs of images describing the microstructures, the properties of constituents, and the mechanical properties of the composites. With these data sets, we train a DNN model to predict the mechanical properties of a composite from a window of its microstructural image. We demonstrate that this DNN model can accurately and efficiently predict the mechanical properties of composites with various complex microstructures, which are difficult to predict with the traditional homogenization methods that use the Eshelby inclusion solution.

In the micromechanics of composites, the RVE concept is widely adopted to estimate the macroscopically effective mechanical responses.[21,22] An RVE should be sufficiently large to avoid significant dependence of the numerical results on its sizes.[23] Besides, periodic or other appropriately specified boundary conditions should be applied to the RVE. Under loading, the total elastic strain energy U stored in the RVE is expressed by

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