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Keynote Paper

Bioinspired Structural Materials: Modeling, Design and Machine Learning

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ABSTRACT

Biological structural materials, which have risen from billions of years of evolution, have developed superior performance of mechanical properties. Distinct from engineering materials, which are unable to perform both lightweight and high strength; high stiffness and high toughness, biological structural materials are often composites of hard/brittle minerals and soft/ductile proteins arranged into complex hierarchical structures which possess remarkable mechanical properties, combining lightweight, high strength and high toughness owing to strengthening and toughening mechanisms from nano-, micro-, meso-, and macro-scales. In this paper, a generalized nacre-inspired composite is modeled and analyzed to explore toughening mechanism inspired by the Nature. To compute the effective properties of the microstructures, an image-based Fast Fourier Transform (FFT) for micromechanics is introduced. A classification criterion based on microcrack length is developed to identify brittle, ductile and toughening behavior of materials. Finally, the dataset from simulation is used to train a machine learning model that results in 91% of accuracy in predicting the desirable materials behavior.

1. INTRODUCTION

Bioinspired structural materials arrange hard and soft materials in complex structures to create unique combinations of strength and toughness, mimicking what researchers observed in the Nature (Barthelat & Mirkhalaf, 2013; Bouville et al., 2014; Jäger & Fratzl, 2000; Wegst et al., 2015). Due to its superior mechanical performance, many studies focus on the brick-and-mortar structure and its mechanism (Barthelat, 2010; Begley et al., 2012; Evans et al., 2011; Gao et al., 2003; Wang et al., 2011). A main conclusion drawn from these studies is that the growth of microcracks is a key factor for the superior toughening mechanism (Huang et al., 2018; Mayer, 2005).

In this study, the composite structure inspired by nacre is generalized to explore the design space of toughening mechanisms. Proper selection of design parameters is identified. Image-based analysis and machine learning model are developed to explore brittle, ductile and toughening behavior of materials by design.

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2. MODELING

To explore the design space of toughening mechanisms, the computational method and design parameters need to be considered carefully. In this study, Fast Fourier transform for micromechanics (FFT) is exploited as the computational method (Moulinec & Suquet, 1998) and the exploring space is chosen followed the concept of Barthelat & Mirkhalaf (2013).

2.1 Computational Method

Fast Fourier transform for micromechanics (FFT) is a pixel-based method. It can directly use image as the mathematic model without further discretization. The main idea of FFT (Moulinec & Suquet, 1998) is turning a heterogeneous problem into a homogeneous problem subjected to a body force (Fig. 1), so that the equilibrium (Eq. (1)) can be rewritten in a convolution form (Eq. (2)) by a periodic Green operator. The solution can then be obtained rapidly in Fourier space.

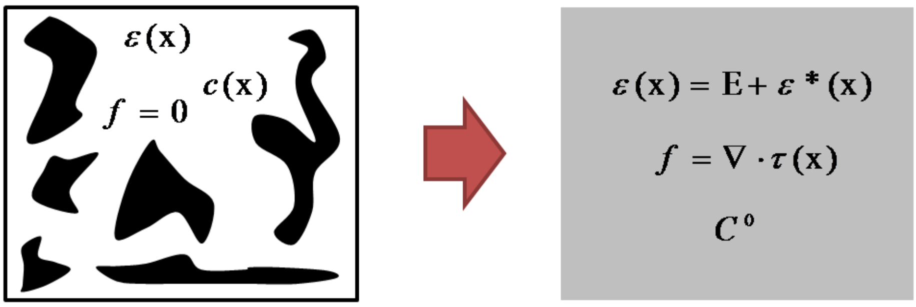

Fig. 1 FFT turns a heterogeneous problem into a homogeneous problem subjected to a body force. (Huang et al., 2018)

$$\nabla \cdot \sigma(x) = \nabla \cdot \Big(\big(C^0(x) : \varepsilon(x) \big) + \tau(x) \Big) = 0 \tag{1}$$

$$\varepsilon\big(u^*(x)\big) := \bar{\varepsilon} - \int \Gamma^0(x,\xi) : \tau(\xi) d\xi \tag{2}$$

To describe the behavior of microcracks, we introduce non-local damage model (Li, Meng, et al., 2012; Li, Tian, et al., 2012) which takes the weighted average near the crack to avoid a direct calculation of stress singularity (Eq. (3)).

$$\hat{\sigma}_e(x) = \frac{1}{\int_V \; w(x-y)dy} \int_V \; w(x-y)\sigma_e(x)dV \tag{3}$$

More details of the computational method mentioned above can be found in Huang et al. (2018).

2.2 Model Setting

Inspired by nacre, the considered model should include brick-and-mortar structure. Meanwhile, to explore the design space with reasonable cost of computational efforts, design parameters need to be chosen carefully. This study exploits the topology shown in Fig. 2, setting the geometry parameters as:

$$H = [32, 64, 128],\ L = 128,\ Ha = Hc,\ La = Lc$$
$$Hb = [1, H/4, H/2, H\text{-}2],\ Lb = [1, L/4, L/2, L\text{-}2]$$

These parameters are chosen to study the extreme cases (Hb = 1, H-2) and difference of the aspect ratios (H = 32, 64, 128; Hb = H/4, H/2). Notice that the size 128 is chose to assemble the structure into 256x256, which is the most common size for image recognition. Total 5,664 cases are considered herein.

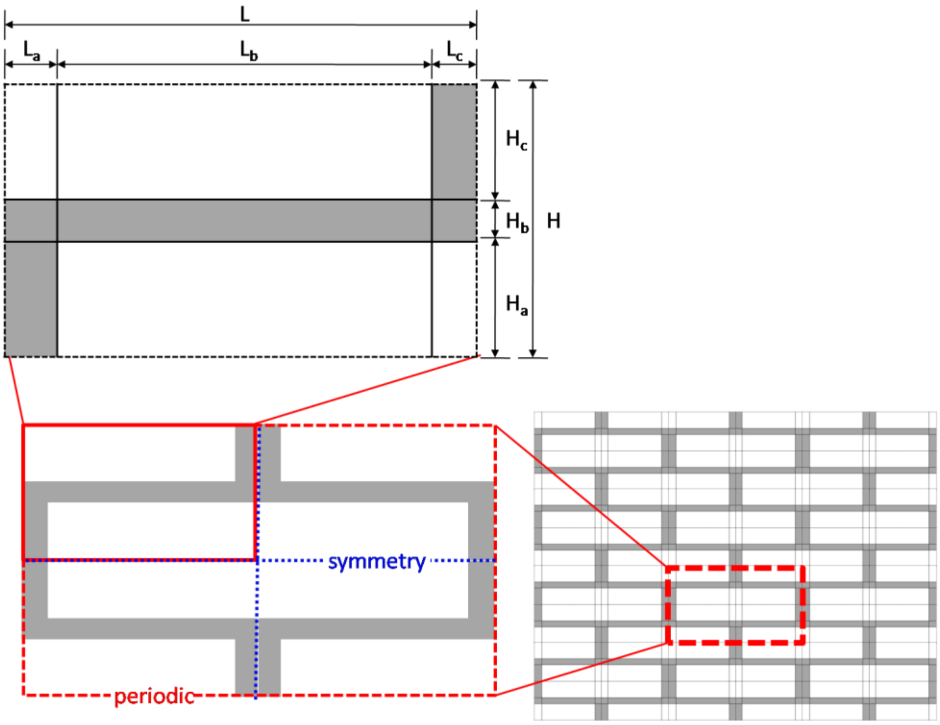

Fig. 2 Geometry parameters and the relation between topology and periodic microstructures. (Barthelat & Mirkhalaf, 2013)

3. RESULTS

The 5,664 cases are classified into three types: brittle, ductile and toughening behavior. These results are collected as training and testing dataset for machine learning.

3.1 Classification

Microstructures are classified by the ability of bearing more stress and strain after cracking (Fig. 3). Three distinct types are classified, including brittle (type I, in green lines), ductile (type II, in blue lines) and toughening (type III, in red lines). In short, type I behaves as the component material which is a typical brittle material and the structure of this type cannot bear any more stress or strain after cracking. Type II can bear more strain, but cannot bear any more stress after cracking. Type III, the target of this study, can bear more stress and strain after cracking, which behaves totally different with the component material.

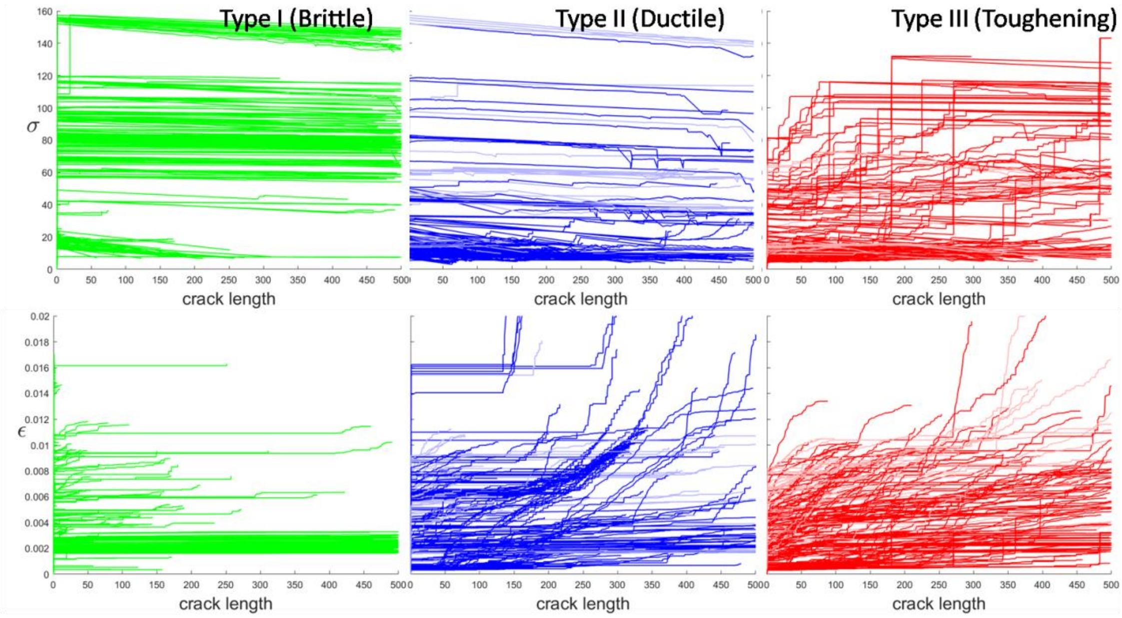

Fig. 3 crack length versus stress and strain of three types structures

3.2 Machine Learning

Using the image as the feature, and type of the structure as label, we build 1,000 samples as the dataset. Fig. 4 shows the result with 80% of the dataset for training and 20% for testing using support vector machine. The accuracy is about 91%. Further enhancement and parameter tuning of the machine learning model is possible and is the subject of future study.

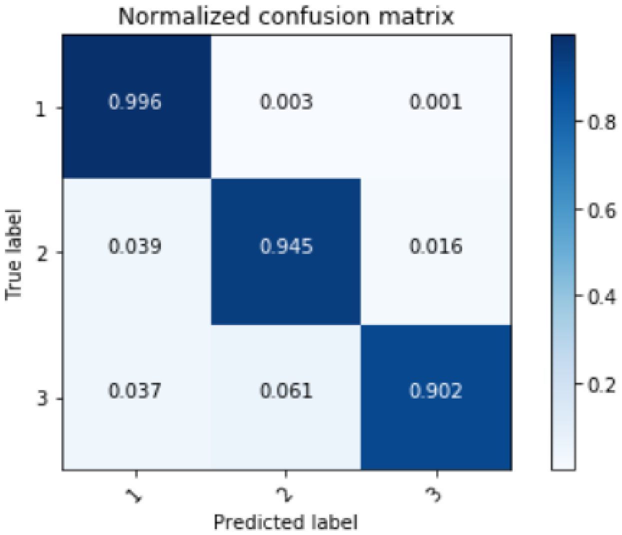

Fig. 4 Results of SVM using 1,000 samples.

4. Conclusions

A generalized design space for composite materials inspired by nacre is investigated. Total 5,664 cases are considered. An image-based Fast Fourier Transform (FFT) is developed to compute the stress-strain response for these cases. A classification criterion based on microcrack length is developed to identify brittle, ductile and toughening behavior of materials. Finally, the dataset from simulation is used to train a machine learning model that results in 91% of accuracy in predicting the desirable materials behavior.

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