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Multi-scale genome modeling for predicting fracture strength of silicon carbide ceramics

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ABSTRACT

The variational asymptotic method for unit cell homogenization (VAMUCH) has emerged as a general purpose micromechanics approach capable of predicting the effective properties of heterogeneous materials and recovering the local fields. In this study, a novel micromechanics approach has been developed enabling VAMUCH to homogenize heterogeneous microstructure and predict its crack formation through a multi-scale materials genome model. A variational form for homogenization is formulated in combination with a cohesive zone model. The weak form of the problem is derived using an asymptotic method, discretized using finite element formulations, and implemented into VAMUCH. The advantages of the present approach are demonstrated through homogenizing silicon carbide ceramics and predicting its fracture strength. Both the elastic properties and fracture strength can be predicted in a computationally efficient manner using this approach compared with the multi-scale finite element model.

1. Introduction

Ceramics and composites are widely used in structural components due to their capabilities of exhibiting desired bending stiffness, fracture strength, or thermal conductivity. Most of them have very complicated microstructure, often accompanied by nonlinear and history-dependent deformation and crack formation. One major challenge is to predict their mechanical behavior from the microstructural details. The computation costs are usually very high if too much microstructural details are considered. On the other hand, their mechanical behavior is strongly affected by the microstructure. A lack of microstructural details in modeling often leads to a large discrepancy between simulations and actual properties. Hence, it is necessary to develop a micromechanics-based predictive model to efficiently predict the mechanical behavior of ceramics and composites.

Several semi-analytical approaches have been developed to homogenize the properties of ceramics or composites with complex microstructures. These approaches often involve finely discretizing a unit cell (UC) or a representative volume element (RVE) that captures the representative periodic microstructure of ceramics or composites. One of the popular semi-analytical approaches is the transformation field analysis (TFA) [1,2], which treats plastic strain as a uniform eigenstrain over each phase and can be implemented in the finite element method (FEM) [3]. Another semi-analytical approach is the method of cells (MOC) or the generalized method of cells (GMC) [4], which discretizes a UC into numerous subcells and approximates the local quantities with their averages over each subcell. However, these approaches can neither accurately handle complex loading conditions [5] nor make very accurate predictions in considering microstructural details and local fields.

Computational approaches have also been implemented based on the finite element analysis. One of the most popular methods is the FEM-based multi-scale method, which arises from the need to understand the material behavior at length scales spanning several orders of magnitude. In particular, the crack formation occurs at a number of length scales, e.g. bond-breaking at the quantum level, interface separation at the nanoscale, micro-crack initiation at the micro-scale, evolution of the micro-cracks into fractures at the macro-scale. An approach was developed to handle the micro–macro transitions in the multi-scale finite element analysis [6], which required kinematic or static boundary conditions at the UC level. An approach using periodic boundary conditions was implemented in the analysis of the UCs of long fiber-reinforced composites [7] and axisymmetric 2D UCs [8] undergoing finite deformation. However, it is challenging to apply periodic boundary conditions because the displacements are not necessarily periodic. When there exists a micro-scale crack [9], periodic boundary conditions, which are often used at the fine-scale to improve convergence, are even more difficult to implement. Under uniaxial and

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biaxial loadings, the periodic boundary conditions were applied to study the damage and failure of the 3D UC of 2D plain weave composites [10]. While the FEM-based homogenization analysis of one RVE can be used to predict effective material properties for the macroscopic analysis, one additional analysis within the local region needs to be performed, e.g., building a sub-model [11], to recover the local fields based on the global response. To overcome this drawback, a variational multi-scale method [12] was developed, where there was no need to use any special interface elements to predict crack propagation in a polycrystalline microstructure. An explicit microstructural representation was introduced to capture microstructure details. A discontinuous displacement field was added to the elements that exceed the damage threshold during loading. While the FEM-based multi-scale method offers the possibility to represent the entire crack geometry, the microstructural effects can be only considered after explicitly modeling the microstructure with fine mesh, which may greatly increase the computational costs.

The variational asymptotic method for unit cell homogenization (VAMUCH) has emerged as a general-purpose micromechanics method that is capable of predicting the effective properties of heterogeneous materials and recovering the local fields with periodic boundary conditions and reduced computational costs [13–18]. It involves a variational analysis of the UC of a composite and asymptotically solving the resulting simplified functional equation governing the response. Its first-order approximation is actually mathematically equivalent to the formal asymptotic homogenization method and thereby possesses similar advantages. Moreover, since both this method and FEM are inherently variational approaches, it is straightforward to implement this method in FEM. Zhang and Yu [18,19] used it to homogenize elasto-viscoplastic heterogeneous composites, and it was further extended to homogenization of elastoplastic composites. However, the crack formation within the heterogeneous microstructure has not been studied.

The objective of the present study is to develop a novel materials genome model to efficiently study the crack formation within heterogeneous materials. While VAMUCH is able to study finite deformation, the introduction of a cohesive zone model in this study enables it to handle crack formation and retains its capabilities in greatly reducing computational costs. The finite element formulation of VAMUCH with a cohesive zone model is derived with the development of the corresponding code structure. The application of this new model is to model crack formation and predict the fracture strength of heterogeneous materials such as ceramics and composites with reduced computational costs. The proposed materials genome model is capable of handling the complex constitutive behavior of different phases of heterogeneous materials under complex loading conditions.

2. Materials genome model with cohesive zone using VAMUCH method

To consider the heterogeneous microstructure of ceramics or composites, a multi-scale genome model is proposed for predicting crack formation. The schematics of the multi-scale ceramic genome model are shown in Fig. 1 for demonstration. It is worth noting that the proposed model can also be extended to model composites. Instead of explicitly modeling every heterogeneous microstructural detail as needed in the conventional finite element analysis, the bulk material is only uniformly meshed as shown in Fig. 1A, with each element representing a materials genome. The heterogeneity will be handled by the materials genome model discussed below. Hence, the computational costs can be greatly reduced as demonstrated in previous studies [13]. However, the

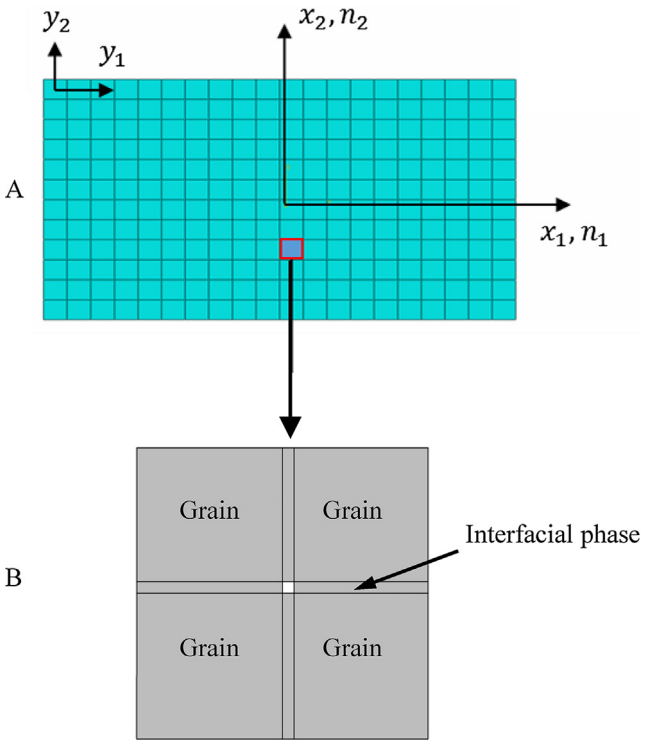

Fig. 1. Illustration of the multi-scale ceramic genome model to predict crack formation: A shows the homogeneous continuum model of bulk materials while B represents the selected genome with a combination of grain and interfacial phase.

previous studies [13,17–19] only investigated the contribution of continuum elements to a materials genome, which are often very difficult to implement in studying crack formation within heterogeneous materials. To account for the crack formation that was not considered in studying the genome of heterogeneous materials [13,17–19], the materials genome model in this study incorporates a cohesive zone model by explicitly including cohesive fracture energy in the framework of VAMUCH.

Each genome is selected based on the typical microstructural characteristics of ceramics [20–26], which mainly consists of grains and interfacial phase as shown in Fig. 1B. Ceramic grains within a genome in Fig. 1B are modeled by continuum elements that represent a cluster of grains with different shapes and sizes. The variation of ceramic shape and size determines the dimensions of the continuum elements. Both the upper and lower limits of the variation are simulated to determine the uncertainties of the prediction results. Different from previous studies [13,17–19], cohesive elements are incorporated to explicitly model the interfacial phase around grains in Fig. 1B and potential crack formation. The thickness of cohesive elements corresponds to the thickness of interfacial phase. It should be noted that although there may exist other minor phases, e.g., secondary phase and defects, they usually only occupy a small portion of ceramics and hence will not significantly affect materials properties. Therefore, to reduce computational costs, only the major phases, i.e., grains and interfacial phase, are included in modeling a materials genome of ceramics.

It is also worth noting that, as uniformly distributed ceramic grains and interfacial phases are implemented, the smallest building block will be sufficient in the analysis of heterogeneous materials [14]. Increasing the dimensions of the genome and including more ceramic grains or interfacial phases will not affect the prediction accuracy of the materials genome model but will only increase the computational costs. Hence, the smallest building block of ceramics is chosen as a genome as shown in Fig. 1B.