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Numerical quantification of the impact of microstructure on the mechanical behavior of particulate Al/SiC composites in 2D

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ABSTRACT

The objectives of the current manuscript are twofold: (i) Introducing an automated computational framework for creating realistic finite element models of metal matrix composites (MMCs) microstructures; (ii) Implementing this technique to investigate the effect of microstructure on the mechanical behavior of an Al/SiC particulate MMC. A microstructure reconstruction algorithm is proposed, which relies on the Centroidal Voronoi tessellation, together with the erosion, random movement, and iterative elimination of the resulting Voronoi cells to create an initial periodic virtual microstructure. Non-Uniform Rational B-Splines are also employed to capture the realistic shapes of embedded particles. High fidelity finite element models of the composite microstructure are then created using a non-iterative Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) technique. This integrated numerical framework is employed to analyze the effect of an Al/SiC MMC microstructure on its mechanical behavior, considering the plastic deformation of the Al matrix and damage in the SiC particles.

1. Introduction

Particle reinforced metal matrix composites (MMCs) are widely used as structural components in aerospace and automotive industries due to their high stiffness, strength-to-weight ratio, and wear resistance (Ayyar and Chawla, 2006; Li et al., 1999). The mechanical behavior of such composites is dependent on their microstructural features such as the volume fraction, shape, and size distribution of reinforcing particles (Segurado et al., 2003; El Moumen et al., 2015). Further, it has been shown that the spatial arrangement of embedded heterogeneities (i.e., uniform distribution versus local clustering) can affect the MMC's plastic and damage responses (Segurado and Llorca, 2006; Deng and Chawla, 2006). Thus, the ability to incorporate the complex microstructure of an MMC in the computational model is essential for the accurate prediction of its mechanical behavior, which is also crucial for the reliable design of corresponding structural components.

In order to characterize the effect of microstructure on the mechanical behavior of composite materials, several micromechanical models and numerical techniques have been developed. To enumerate a few models belonging to the former category, we can mention the Eshelby model (Eshelby, 1957), Hashin–Shtrikman bounds (Hashin and Shtrikman, 1963), and self-consistent estimate (Hill, 1965). Since such micromechanical models do not incorporate the effect of plasticity and damage, they cannot properly predict the strength and toughness of the composite; thus their application is often limited to evaluating linear elastic properties. Instead, one can implement numerical techniques such as the Nonuniform Transformation Field Analysis (NTFA) (Michel and Suquet, 2003; 2004) and the finite element method (FEM) (Segurado et al., 2003; Segurado and Llorca, 2006) to predict the homogenized nonlinear response of the material. For example, Michel and Suquet (2004) implemented the NTFA to evaluate the effective nonlinear mechanical properties of composites. Geni and Kikuchi (1998) used the FEM to conduct damage simulations and quantify the effect of nonuniform spatial distribution of particles on the failure response of an Al matrix composite. Han et al. (2001) employed a statistical description of particle damage to study the effect of spatial arrangement of the embedded heterogeneities on the mechanical behavior of an MMC. Several other studies have been conducted in this field besides the examples enumerated above.

In addition to using appropriate material models, the fidelity of a numerical simulation for predicting the behavior of an MMC depends on incorporating its realistic microstructural features in the computational model. The complex nature of these microstructures leads to two major challenges toward achieving this goal: (i) creating realistic geometrical models of the composite microstructure; (ii) discretizing them using appropriate conforming meshes. In

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theory, the former phase can be accomplished by using sophisticated Computer Aided Design (CAD) software packages or using digital data such as Scanning Electron Microscope (SEM) images. However, the modeling process using such approaches is often laborious, time-consuming, and imposes additional challenges pertaining to image processing (noise filtration Ng and Ma (2006), segmentation (Salembier and Garrido, 2000), etc.). To this end, simulating the micromechanical behavior of composite materials involves other considerations such as periodicity of the representative volume element (RVE) (Young et al., 2008), which further increase the complexity of the modeling process. Such difficulties are further amplified in problems such as Uncertainty Quantification (UQ) (Arbelaez and Zohdi, 2009) and Integrated Computational Materials Engineering (ICME) (Purkayastha and McMeeking, 2012), where multiple models, each with a distinct microstructure, must be created and analyzed throughout the solution process.

In order to alleviate the difficulties mentioned above, several algorithms have been introduced to enable the reconstruction of synthetic microstructures with desired morphological and statistical features. These techniques employ a wide array of algorithms for reconstructing a virtual microstructure, including modified versions of the Random Sequential Adsorption (RSA) (Soghrati and Liang, 2016; Fritzen et al., 2012), Voronoi tessellation (Ghosh et al., 1995; Fritzen et al., 2009), modified Monte Carlo method (Li et al., 2010; Tabei et al., 2013), and stochastic optimization (Yeong and Torquato, 1998; Kumar et al., 2008; Liu et al., 2013). A comprehensive review of varying microstructure reconstruction algorithms is provided in Fullwood et al. (2010). Such algorithms enable the construction of multiple microstructural models with desired features such as the volume fraction and spatial arrangement of particles.

Discretizing a virtual microstructure created using the aforementioned reconstruction algorithms to build an appropriate finite element (FE) model could still be a challenging task (Geuzaine and Remacle, 2009). Several robust mesh generation algorithms (Zhang et al., 2010) have been developed to address this issue, including the Delaunay triangulation method (Shewchuk, 2002), advancing front (Lo, 1985; Schöberl, 1997), and quadtree-based techniques (Yerry and Shephard, 1984). Although these methods can successfully create conforming meshes for problems with complex morphologies, this process involves an iterative smoothing/optimization phase (Baehmann et al., 1987) to minimize the geometric discretization error and improve the elements quality. Apart from the complexity and computational cost associated with such mesh generation algorithms, additional time and labor are often necessary to prepare a virtual microstructure (e.g., by transforming that into a CAD model) before being able to create the mesh.

More FE-based advanced numerical techniques, including the CutFEM (Burman et al., 2015), the extended/Generalized FEM (X/GFEM) (Babuska and Melnek, 1997; Moës et al., 1999; Duddu et al., 2008), and the hierarchical interface-enriched FEM (HIFEM) (Soghrati, 2014; Soghrati and Ahmadian, 2015) have been introduced to avoid the laborious process of creating conforming meshes. In the X/GFEM, the partition of unity method is employed to add appropriate enrichments for simulating strong (field) and weak (gradient) discontinuities in nonconforming elements (Belytschko and Black, 1999; Oden et al., 1998). The HIFEM attaches enrichment functions to the generalized degrees of freedom (DOFs) added at the intersection points of materials interfaces with edges of background elements, to simulate the discontinuous phenomenon. While such techniques are often categorized as mesh-independent methods, it is necessary to subdivide the nonconforming elements into smaller sub-elements (children elements) conforming to the materials interface to accurately perform the numerical quadrature (Oden et al., 1998; Soghrati and Geubelle, 2012). Since such children elements might have exceedingly high aspect ratios, additional treatments are often required to resolve issues such as ill-conditioned stiffness matrices, poor approximation of stress concentrations along materials interfaces, and imposing Dirichlet boundary conditions (Belytschko et al., 2009; Soghrati, 2014).

Recently, Soghrati et al. (2017) have introduced a Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) technique, which enables the construction of high-quality conforming meshes using a straightforward non-iterative algorithm. The CISAMR automatically transforms a structured grid into a conforming mesh, while ensuring that the element aspect ratios are lower than three in 2D problems. One of the key advantages of this method, which is used for creating the FE models of an MMC in the current manuscript, is the ability to handle problems with intricate morphologies without the need for using an iterative scheme for improving the mesh quality. Thus, the complexity and computational cost associated with the implementation of CISAMR are comparable to the process of creating children elements in mesh-independent methods such as the X/GFEM and HIFEM. Moreover, CISAMR eliminates the need for using enrichment functions in the approximate field by maintaining a high quality mesh, which also reduces the complexity of the algorithm and the total number of DOFs.

The main objectives of this article are twofold: (i) Introducing an automated computational framework for creating realistic virtual microstructures and their high fidelity FE meshes, by integrating the CISAMR with a new microstructure reconstruction algorithm; (ii) Employing the proposed framework to investigate the impact of microstructure on the mechanical behavior of a silicon carbide (SiC) particle reinforced aluminum (Al) composite. The proposed microstructure reconstruction algorithm enables the creation of realistic periodic RVEs of MMCs with the desired shape, volume fraction, size distribution, and spatial arrangement of the embedded particles. We then implement the CISAMR to convert generated microstructural models into appropriate conforming meshes for FE analyses. One of the main objectives of this integrated computational framework is to provide an easy-to-implement algorithm for creating microstructural models for MMCs with intricate microstructures, without sacrificing the robustness and fidelity. In order to predict the mechanical behavior of the Al/SiC MMC studied in this work, we use an isotropic continuum brittle damage model (Matouš et al., 2008) to simulate the damage process in the SiC particles. We also implement a plane stress-projected plasticity model (Simo and Taylor, 1986) to simulate the nonlinear mechanical behavior of the Al matrix.

2. Problem formulation

2.1. Micromechanical model

Consider an open domain Ω with the boundary $\partial\Omega = \Gamma$ and outward unit normal vector $\mathbf{n}_{\mathrm{M}}$ representing an Al/SiC particulate composite panel in the macroscopic coordinate system $\mathbf{x}_{\mathrm{M}}$. Also, assume an open domain Θ with the boundary $\partial\Theta = \Lambda$ and outward unit normal vector $\mathbf{n}_{\mathrm{m}}$ corresponding to a microscopic RVE of this MMC defined in the microscopic coordinate system $\mathbf{x}_{\mathrm{m}}$. When subject to macroscopic mechanical loads, the macroscopic and microscopic displacement fields, i.e., $\mathbf{u}_{\mathrm{M}}(\mathbf{x}_{\mathrm{M}})$ and $\mathbf{u}_{\mathrm{m}}(\mathbf{x}_{\mathrm{m}})$, respectively, can be linked together via a first-order asymptotic expansion of the total displacement field $\mathbf{u}(\mathbf{x}_{\mathrm{M}}, \mathbf{x}_{\mathrm{m}})$ as

$$\mathbf{u}(\mathbf{x}_{\mathrm{M}}, \mathbf{x}_{\mathrm{m}}) = \mathbf{u}_{\mathrm{M}}(\mathbf{x}_{\mathrm{M}}) + \mathbf{u}_{\mathrm{m}}(\mathbf{x}_{\mathrm{m}}). \tag{1}$$

The strong form of the governing equations describing the response of Θ subject to macroscopic strain $\boldsymbol{\varepsilon}_{\mathrm{M}}$ can be expressed as: