Analyzing the impact of microstructural defects on the failure response of ceramic fiber reinforced aluminum composites

Hossein Ahmadian\textsuperscript{a}, Bowen Liang\textsuperscript{a,c}, Soheil Soghrati\textsuperscript{a,h,c,}\textsuperscript{*}
\textsuperscript{a} Department of Mechanical and Aerospace Engineering, The Ohio State University, USA
\textsuperscript{b} Department of Materials Science and Engineering, The Ohio State University, USA
\textsuperscript{c} Simulation Innovation and Modeling Center (SIMCenter), Columbus, Ohio, USA

ABSTRACT

The computational homogenization technique is employed to investigate the effect of pre-existing microstructural voids on the failure response of a ceramic fiber reinforced aluminum composite subjected to loads in transverse to the fiber direction. Automated numerical simulations are carried out using a hierarchical interface-enriched finite element method (HIFEM), which enables the use of simple structured meshes for creating the discretized model. The HIFEM is integrated with a new microstructure quantification algorithm relying on the Random Sequential Adsorption (RSA) and Non-Uniform Rational B-Splines (NURBS) to create realistic periodic unit cells of the composite based on imaging data. A strain-driven homogenization problem is then solved at the microscale to simulate the damage evolution in the aluminum matrix using the Lemaitre elasto-plastic damage model. Six virtual models of the composite microstructure with varying volume fractions and spatial distributions of pre-existing voids are analyzed to determine their failure responses subject to macroscopic normal and shear strains. The outcomes of this study indicate that although for the latter type of loading the impact of small volume fractions of voids on the failure response is negligible, their presence significantly deteriorates the composite mechanical strength subject to uniaxial and equi-biaxial macroscopic normal strains.

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1. Introduction

By providing light-weighting and high strength-to-weight ratio, aluminum-based metal matrix composites (MMCs) are highly suited for aerospace and automotive applications (McDanel, 1985; Tjong and Ma, 2000). Reinforcing the aluminum matrix with a ceramic phase such as Al₂O₃ could not only improve the strength of the resulting composite material but also provide superior thermal properties required for automotive and aerospace applications (Kainer, 2006; Rawal, 2001; Surappa, 2003). The performance of the resulting composite materials system is highly dependent on its microstructure, which is governed by parameters such as the volume fraction of embedded fibers, their morphologies, and spatial/size distribution (Chawla, 2012; Torquato, 1998). Further, it is important to quantify the impact of microstructural defects such as pre-existing voids on the mechanical behavior of the MMC (Becker, 1987; Soppa et al., 2003). Note that the presence of such microstructural voids is practically inevitable in many types of MMCs due to either manufacturing constraints or the unjustifiably high cost associated with eliminating them. Moreover, the random distribution of defects in the MMC microstructure leads to uncertainty in its mechanical behavior, which makes it more challenging to accurately quantify their impact on the failure response of this composite material.

The objective of the current manuscript is to quantitatively understand the effect of pre-existing voids on the failure response of ceramic fiber reinforced aluminum composite thin films (prepregs) used in the Ultrasonic Additive Manufacturing (Graff, 2011; Hopkins et al., 2012) of multi-ply MMCS. This study is motivated by a significant inconsistency observed in the experimental measurements and analytical assessments of the prepreg mechanical strength when subjected to loads in transverse to the fiber direction. After preparing X-ray micro-computed tomography (micro-CT) images of the composite microstructure, several pre-existing voids oriented in the longitudinal fiber direction were identified in the aluminum matrix. In this work, we test the hypothesis that the presence of these elongated voids has a considerable impact on reducing the mechanical strength of the MMC.
Several studies have been carried out to understand the effect of embedded heterogeneities on the failure response of MMCs (Ayyar et al., 2008; Drabek and Böhlm, 2006; Mishnaevsky, 2006; Mishnaevsky et al., 2004; Qing, 2013). However, less emphasis has been put on quantifying the impact of manufacturing flaws and more importantly the uncertainty emanating from their presence on the material response using numerical techniques. To name a few works in this field, we can mention the numerical model presented in Soppa et al. (2003) for investigating the effect of residual stresses on the failure of Al-Al₂O₃ composites, a homogenization-based continuum damage model for evaluating the ductile failure of MMCs in Ghosh et al. (2009), the elastoplastic damage model proposed in Pyo and Lee (2010) considering the effect of imperfect interface in fiber reinforced metal matrix composites, and the statistical model introduced in Kim (2006) to investigate the impact of voids size distribution on the tensile deformation response of SiC particulate-reinforced aluminum composites.

Quantifying the failure response of the MMC studied in this article requires the ability to create realistic computational models of the material microstructure with varying volume fractions and spatial/size distributions of pre-existing voids. The first step of this process is to build multiple geometrical models of the MMC heterostructure, which is clearly not possible via computer-aided design (CAD) tools due to the complexity of the microstructure (Beall et al., 2003). Another option would be the direct transformation of digital data such as Scanning Electron Microscopy (SEM) or micro-CT images into a conforming mesh to perform finite element method (FEM) simulations (Reid et al., 2008; Young et al., 2008). However, given the requirement to capture multiple permutations of pre-existing voids in the material microstructure to quantify the uncertainty induced by their presence on the MMC’s mechanical behavior, it is also not feasible to implement this approach due to the costly and laborious process of imaging and image processing (noise filtration, segmentation, etc.) (Sonka et al., 2014).

To alleviate this limitation, several researchers have developed synthetic microstructure reconstruction algorithms for creating virtual models of composite microstructure based on information extracted from imaging data (e.g., morphology, volume fraction, and spatial distribution of embedded particles) (Fullwood et al., 2010; Marur, 2010). For instance, several algorithms relying on the Random Sequential Adsorption (RSA) (Fritzen et al., 2012; Soghriati and Liang, 2016), Voronoi tessellation (Ghosh et al., 2001; Said et al., 2016; Wimmer et al., 2016), and N-point statistics (Fullwood et al., 2008; Niezgoda et al., 2010) have been developed for creating virtual models of heterogeneous materials. In this work, we implement a modified version of the algorithm introduced in Soghriati and Liang (2016) for creating multiple plane strain models of the Al/Al₂O₃ MMC by integrating the RSA algorithm and Non-Uniform Rational B-Splines (NURBS) (Piegl and Tiller, 2012). It must be noted that the effect of residual stresses induced during the manufacturing process, which requires using a generalized plane strain model (González and Llorca, 2007; Schmauder et al., 2003; Taliercio, 2005) for more accurate evaluation of the failure response, is not taken into account in the current study. Further, the plane strain assumption used in the current manuscript is valid provided that the microscopic model corresponds to a microscopic point away from edges of the composite panel, as out-of-plane strains could violate this assumption in such regions (Reusch et al., 2008).

Another major step involved in simulating the MMC failure response is to transform the virtual microstructures into finite element (FE) models, which requires constructing appropriate conforming meshes (Behr and Tezduyar, 2001; Frey and George, 2010). Due to the complexity of the MMC microstructure, creating such meshes for multiple permutations of the volume fraction and spatial distribution of pre-existing voids is a challenging and time-consuming task. To address this challenge, one could implement mesh-independent numerical techniques such as the element free Galerkin method (EFGM) (Belytschko et al., 1994; Nguyen et al., 2008), the generalized interface-enriched FEM (IGFEM) (Aragón et al., 2013; Soghriati et al., 2012; Soghriati and Guebels, 2012), or the eXtended/Generalized FEM (X/GFEM) (Belytschko and Black, 1999; Melnek and Babuska, 1996; Moës et al., 1999; Oden et al., 1998) to eliminate the requirement of using conforming meshes. The latter two methods achieve this objective by enhancing the solution field in nonconforming elements by adding appropriate C₀-continuous enrichment functions that can accurately simulate gradient discontinuities (e.g., in the stress field) along materials interfaces. In this article, we implement the hierarchical interface-enriched FEM (HIFEM), originally introduced by Soghriati (2014) and further expanded in Soghriati and Ahmadian (2015); Soghriati and Barrera (2016), to simulate the MMC mechanical behavior using simple structured meshes for creating the discretized models. The HIFEM implements a hierarchical enrichment strategy to capture the discontinuous phenomena, which can easily handle fiber/void/matrix interfaces that are in close proximity, contact, and even intersecting with one another.

Simulating the damage process in the MMC microstructure also requires an appropriate physics-based model to describe the initiation and evolution of damage in the aluminum matrix. While from the microscopic point of view, the damage in ductile materials is associated with nucleation, growth, and coalescence of voids (not to be confused with pre-existing voids or defects), the macroscopic effect of damage is the reduction of the stiffness, strength, and toughness of the material (Xue, 2007). Accordingly, continuum damage models developed for simulating the elasto-plastic damage response of ductile materials can be divided into two main categories (Ju, 1989; Simo and Ju, 1987): (i) microscopic models, such as the Gurson model (Gurson, 1977; Pardoien and Hutchinson, 2000; Thomson, 1993), which aim at simulating the damage process by homogenizing the void growth process in repeating unit cells (RUCs) of the material (Chabanet et al., 2003; Verhoosel et al., 2010); (ii) macroscopic or phenomenological models, which rely on thermodynamic laws for simulating the damage evolution. The Lemaitre ductile damage model (Lemaitre, 1985a, 1985b), which belongs to the second category, is implemented to simulate the MMC failure response in this work.

The remainder of this manuscript is structured as follows: In Section 2, we present the governing equations and the Lemaitre ductile damage model formulation for simulating the MMC failure response. Section 3 introduces the automated framework developed for creating computational models, which includes the mesh-independent HIFEM solver and an image-based microstructure quantification algorithm for creating realistic virtual models of the composite microstructure. The appropriate size of the RUC for performing damage simulations is identified in Section 4. In Section 5, we present the results of numerical simulations and investigate the impact of pre-existing voids on the failure response of the MMC subject to macroscopic normal and shear strains. Final concluding remarks are provided in Section 6.

2. Problem formulation

2.1. Computational homogenization approach

Consider an open domain \( \Omega \subset \mathbb{R}^2 \) representing a microscopic RUC of the MMC with three mutually distinct sub-regions \( \Omega = \Omega_m \cup \Omega_f \cup \Omega_r \) corresponding to the aluminum matrix, ceramic fibers, and pre-existing voids, respectively. The domain boundary \( \partial \Omega = \Gamma \) has an outward unit normal vector \( \mathbf{n} \) and periodic boundary conditions along all edges, meaning that displacement vectors corresponding to mesh nodes on two parallel edges of \( \Omega \) with
either similar $x$ or $y$ coordinates are identical. Note that unlike the mathematical homogenization, which requires the global periodicity condition for evaluating the effective properties of the material, the microstructure must only be locally periodic in computational homogenization (Nguyen et al., 2008). Using the first-order homogenization approach (Kouznetsova et al., 2001), the displacement field $u$ of $\Omega$ can be decomposed into a macroscopic displacement field $u_M$ and a microscopic fluctuation field $u_m$, i.e.,

$$u = u_M + u_m. \quad (1)$$

Assuming that $\Omega$ is subjected to a macroscopic strain tensor $\varepsilon_M$, the strong form of the linear elastic governing equations in $\Omega$ is expressed as: Find the microscopic displacement field $u_m$ such that

$$\begin{cases}
\nabla \sigma_m = 0 & \text{in } \Omega_1 \\
\sigma_m = C_\varepsilon (\varepsilon_M + \varepsilon_m) & \text{in } \Omega_1 \\
\varepsilon_m = \frac{1}{2} \nabla u_m + \nabla u_m^T & \text{in } \Omega_1,
\end{cases} \quad (2)$$

where $\varepsilon_m$ is the microscopic strain tensor, $\sigma_m$ is the microscopic Cauchy stress tensor, and $C_\varepsilon$ is the fourth-order elasticity tensor associated with the $i$th material phase.

The weak form of (2) can be approximated by selecting $u_m$ from a set of admissible displacement functions $\tilde{u}$ such that

$$u_m \in \tilde{u} := \left\{ \mathbf{v} : \tilde{\Omega} \rightarrow \mathbb{R}^2 \subset H^2(\Omega_1) \right\}, \quad (3)$$

where $H^2$ is the second-order Hilbertian Sobolev space. The weak form of the problem is then written as: Find $u_m \in \tilde{u}$ such that

$$\int_{\Omega} \left[ \frac{\partial u_m}{\partial x} 0 \frac{\partial u_m}{\partial x} \frac{\partial u_m}{\partial y} \frac{\partial u_m}{\partial y} \right]^T \mathbf{C} \left[ \begin{array}{c} \frac{\partial v}{\partial x} \\ 0 \\ \frac{\partial v}{\partial y} \end{array} \right] d\Omega = 0 \quad \forall \mathbf{v} \in \tilde{u}. \quad (4)$$

The Galerkin FEM approximation of (4), which is denoted by $u_h$, is evaluated by using the subset $\tilde{u}^h \subset \tilde{u}$ composed of the standard Lagrangian shape functions defined in each element.

The average macroscopic stress $\sigma_M$ in $\Omega$ can be evaluated based on the Hill–Mandel macro-homogeneity principle (Hill, 1985), which requires the free energy density $\Psi_M$ of a macroscopic point to be equal to the average microscopic free energy $\Psi_m$ of $\Omega$, i.e.,

$$\inf_{u_u} \Psi_M(u_M) = \sup_{\varepsilon_u} \inf_{u_u} \frac{1}{|\Omega|} \int_{\Omega} \Psi_m (\varepsilon_u(u_M)) + \nabla u_m \right) d\Omega. \quad (5)$$

Applying standard variational principles to (5) and noting that the microscopic displacement field $u_m$ makes no contribution to the average macrostructural energy (Kouznetsova et al., 2002), $\sigma_M$ can be computed as Kouznetsova et al. (2001); Soghraei and Liang (2016)

$$\sigma_M = \frac{1}{|\Omega|} \int_{\Omega} \sigma_m d\Omega. \quad (6)$$

It must be noted that although only linear elastic governing equations were presented in this section, inelastic mechanical behaviors such as plasticity and damage, which are covered in the following section, are also taken into account for evaluating $\sigma_m$.

### 2.2. Damage model

To simulate the plastic behavior and damage accumulation in the aluminum matrix, we implement the isotropic Lemaitre elasto-plastic damage model, which is formulated based on the assumption of the homogeneous distribution of micro-voids in the damaged state. Using the strain equivalence hypothesis, the strain response of the damaged material can be evaluated by replacing the actual microscopic stress $\sigma_m$ with an effective stress $\sigma_{\text{eff}}$ in the constitutive equations of the undamaged material as de Souza Neto et al. (2008)

$$\sigma_{\text{eff}} = \frac{\sigma_m}{1 - D}. \quad (7)$$

where $D$ is a scalar variable ranging from 0 (undamaged) to 1 (fully damaged) indicating the magnitude of damage. Assuming that the elastic-damage and plastic hardening phenomena are decoupled, the total microscopic free energy of the material can be written as the sum of free energies contributed by each phenomenon, i.e.,

$$\Psi_m = \Psi_{\text{ed}} (\varepsilon^e, D) + \Psi_p (R), \quad (8)$$

where $\varepsilon^e = \varepsilon_0^e + \varepsilon^p$ is the elastic strain tensor and $R$ is a scalar internal variable associated with the hardening process.

The elastic–damage potential in (8) is given by

$$\Psi_{\text{ed}} (\varepsilon^e, D) = \frac{1}{2\rho} \varepsilon^e : (1 - D)\varepsilon^e : \varepsilon^e. \quad (9)$$

where $\rho$ is the density of the material. The constitutive equation of the damaged material is then expressed as

$$\sigma_m = \rho \frac{\partial \Psi_m}{\partial \varepsilon^e} = (1 - D)\varepsilon^e : \varepsilon^e. \quad (10)$$

Also, the thermodynamic force conjugate to the damage parameter $D$ is expressed as

$$Y = \rho \frac{\partial \Psi_m}{\partial D} = -\frac{1}{2} \varepsilon^e : \varepsilon^e. \quad (11)$$

Note that $Y$, also known as the damage energy release rate, relates to the variation of the internal energy density due to the damage growth at a constant stress, which can be evaluated as

$$Y = \frac{-q^2}{6G(1 - D)^2} - \frac{p^2}{2K(1 - D)^2}. \quad (12)$$

In this equation, $p$ is the hydrostatic stress, $q$ is the effective von-Mises stress, and $G$ and $K$ are the shear and bulk moduli, respectively. The plastic free energy $\Psi_p (R)$ is a function of the hardening internal variable $R$, for which the corresponding thermodynamic force is given by

$$\kappa (R) = \rho \frac{\partial \Psi_p (R)}{\partial R}. \quad (13)$$

To satisfy the second principle of thermodynamics, the governing equations for the evolution of internal variables $D$ and $R$ are derived from a microscopic dissipation potential function $\phi_m$. By restricting the formulation to isotropic materials, $\phi_m$ can be approximated as

$$\phi_m = \phi_{\text{ed}} + \phi_p, \quad (14)$$

where $\phi_{\text{ed}}$ is the elastic-damage potential and $\phi_p$ is the plasticity potential (yield function). These potential functions are written as

$$\phi_{\text{ed}} = \frac{r}{(s + 1)(1 - D)} \left( \frac{Y}{r} \right)^{s+1}, \quad \phi_p = [q - \sigma_{y0} - \kappa (R)]. \quad (15)$$

where $\sigma_{y0}$ is the yield stress and $s$ and $r$ are scalar material properties. To ensure the quasi-saturation of the strain hardening when damage occurs, the thermodynamic force is represented by an exponential function, which is written as

$$\kappa (R) = R \delta [-1 - \exp(-bR)]. \quad (16)$$

where $b$ and $R_\delta$ are material constants associated with the plastic yield surface. The evolution laws can then be derived as

$$\dot{\varepsilon}^e = \gamma \frac{\partial \phi_m}{\partial \sigma}, \quad \dot{R} = \lambda \frac{\partial \phi_m}{\partial \kappa}, \quad \dot{D} = \lambda \frac{\partial \phi_m}{\partial Y}. \quad (17)$$

where $\dot{\varepsilon}$ and $\lambda$ are the plastic strain and plastic multiplier, respectively.
To solve the governing equations of the Lemaitre damage model in an FEM-based formulation, we implement the elastic predictor/return mapping algorithm provided in de Souza Neto et al. (2008). Further, to reduce the mesh dependency effects common to all continuum damage models, a nonlocal regularization algorithm similar to that presented in Bazant and Jirásek (2002) is implemented. Nonlocal models are based on choosing an a priori value for the size of the damaged zone for each integration point and then utilizing a weight function to include the effects of other integration points in that zone. Thus, the goal is to replace the local value of the damage with its nonlocal value in a region $V_{AL}$ within the aluminum matrix, which can be written as

$$\tilde{D}(x) = \int_{V_{AL}} \alpha(x, \xi) D(\xi) d\xi$$

where $\tilde{D}$ and $D$ are the nonlocal and local damage variables, respectively. Moreover, $\alpha(x, \xi)$ is a weight function that depends on the distance between the source point $\xi$ and the target point $x$, i.e., $r = |x - \xi|$. This weight function can be evaluated as

$$\alpha(x, \xi) = \frac{\alpha_0(r)}{\int_{V_{AL}} \alpha_0(r) d\xi}$$

where $\alpha_0(r)$ determines the shape of function, which must monotonically decrease with distance $r$. In the current manuscript, we employ a Gauss distribution function (Bazant and Jirásek, 2002) given by

$$\alpha(r) = \exp\left(-r^2 \frac{1}{4\ell^2}\right)$$

where $\ell$ is the so-called internal length scale of the continuum damage model. In this work, $\ell$ is selected such that the internal length scale is twice the size of elements of the structured mesh used for creating the HIFEM models.

3. Automated construction of computational models

3.1. Mesh-independent HIFEM algorithm

A brief overview of the HIFEM formulation (Soghrati, 2014), together with the required considerations for the implementation of higher-order elements and numerical quadrature in this method are provided in this section. Using a structured mesh for discretizing the microscopic RUC, the HIFEM approximation of the displacement field $u^h$ is given by

$$u^h = \sum_{i=1}^{n} N_i u_i + \sum_{j}^{n_m} s_j \Psi_j \alpha_j^{(h)}$$

where $N_i$ is a set of $n$ Lagrangian shape functions, $\Psi_j^{(h)}$ is a set of $n_m$ enrichment functions, $u_i$ is the displacement vector at node $i$ of the mesh, and $\alpha_j^{(h)}$ is the $j$th generalized degree of freedom created at the intersection point of the $h$th materials interface with edges of the nonconforming background element (Fig. 1). The enrichment function $\Psi_j^{(h)}$ in the second term of (21) enables re-constructing weak discontinuities that emanate from the mismatch between material properties across the interfaces between matrix, fibers, and voids in the MMC microstructure. Also, the scalar scaling factor $s_j^{(h)}$ in (21) is associated with the $j$th enriched node of a child element at the $h$th level of hierarchy, which is evaluated as

$$s_j^{(h)} = \sqrt{\min(d_{ij}) \frac{1}{h_r}},$$

where $h_r$ is the size of the root element and $d_{ij}$ is the distance between node $j$ and the $i$th edge of the child element, as shown in Fig. 1b. As explained in more detail in Soghrati et al. (2015), $s_j^{(h)}$ is incorporated in the HIFEM formulation to ensure the construction of a well-posed stiffness matrix that is not affected by enrichment functions associated with children elements with exceedingly high aspect ratios.

The enrichment functions associated with a nonconforming element in the HIFEM are constructed independently for each materials interface intersecting with its edges using a hierarchical approach, which is schematically shown in Fig. 1. In this recursive algorithm, the children elements created for the first materials interface cutting the parent element edges are labeled as the first level of hierarchy (Fig. 1b). These children elements then serve as parent elements for the second materials interface (Fig. 1c) intersecting with the original parent (root) element. This hierarchical discretization scheme is continued until all materials interfaces are visited. The resulting children elements and interface nodes are stored in a tree data structure, in which elements of the original structured mesh can be regarded as roots of the tree and children elements created at the highest level of hierarchy correspond to its leaves. The total enrichment function in a nonconforming element cut by $n_{th}$ materials interfaces can then be evaluated as Soghrati (2014)

$$\Psi_{\text{total}} = \sum_{h=1}^{n_{th}} \sum_{j=1}^{n_h} N_j,$$

where $n_{th}$ also refers to the number of hierarchical levels, $n_h$ is the number of interface nodes at the $h$th level of hierarchy, $n_h$ is the number of children elements connected to the enriched node $j$ at this level, and $N_j$ is the $r$th Lagrangian shape function of the $k$th child element sharing node $j$. Using a recursive algorithm, the hierarchical enrichment scheme given in (23) can easily be applied to elements cut by multiple materials interfaces; thus can handle materials interfaces that are in close proximity or intersecting with one another.

The implementation of higher-order elements in the HIFEM requires further considerations for the construction of a well-posed stiffness matrix and to ensure that similar polynomial orders are used for basis/enrichment functions of both the parent and children elements (Soghrati and Barrera, 2016). To achieve this, the generalized degrees of freedom (dofs) located on edges of children elements that overlap with one of the edges of the parent element (Fig. 2) are constrained to eliminate the redundant dofs causing the ill-conditioning of the stiffness matrix. In Fig. 2, the enriched dofs $\alpha_j^{(1)}$ and $\alpha_j^{(2)}$ associated with the enriched nodes located on the right edge of the six-node triangular parent element are constrained as

$$\alpha_j^{(1)} = \frac{L_j^{(1)}}{2(L_j^{(1)} - L_j^{(2)})} \alpha_j^{(2)},$$

where distances $L_j^{(1)}$ and $L_j^{(2)}$ are depicted in Fig. 2. It must be noted that the constraint (24) is set such that the enrichment function associated with each level of hierarchy vanishes at the edge node of its parent element.

Finally, the hierarchical scheme employed for accurate numerical integration of the $C^0$-continuous enrichment functions during the construction of the stiffness matrix is schematically depicted in Fig. 3. In this algorithm, the numerical quadrature begins from children elements belonging to the highest level of hierarchy (leaves of the tree data structure). The Gauss points created in the local coordinate system of these children elements are then mapped to local coordinates of their parent elements via an inverse isoparametric mapping and this process is recursively continued to reach the root element and evaluate the contribution of basis functions at all levels of hierarchy to the stiffness matrix.
Fig. 1. Hierarchical process of sub-triangulating a nonconforming root element and constructing the HIFEM children: (a) root element cut by two materials interfaces; (b,c) children elements and interface nodes created at the first and second levels of hierarchy, respectively.

Fig. 2. Variation of a second-order enrichment function along the right edge of the parent element after constraining generalized dof \( u_i^{(1)} \) and \( \alpha_j^{(1)} \) to one another.

Second level of children elements

First level of children elements

Non-conforming parent element

Gauss point

\( (\xi^{(2)}, \eta^{(2)}) \)

\( (\xi^{(1)}, \eta^{(1)}) \)

\( (\xi^{(0)}, \eta^{(0)}) \)

3.2. Image-based microstructure quantification

The HIFEM simulation of the MMC mechanical behavior requires the ability to create multiple microstructural models of the composite with varying volume fractions and spatial distributions of voids. To accomplish this, we implement a new microstructural quantification algorithm (Soghrati and Liang, 2016) and integrate with the HIFEM to automatically generate synthetic microstructural models of the composite based on imaging data, as schematically shown in Fig. 4. The first step is to carry out the required image processing tasks on the micro-CT data to identify different materials interfaces, as shown in Fig. 4a. Fig. 4b illustrates a cross section of the MMC microstructure, which clearly shows the presence of pre-existing voids. Note that in order to use a plane strain model to simulate the failure response of this MMC, the voids must have a much longer characteristic length in the longitudinal direction of ceramic fibers. Fig. 5a, which illustrates the 3D architecture of pre-existing voids, verifies such an arrangement and thus the feasibility of using a plane strain model. Note that the morphology of these voids in the MMC microstructure is very different than typical ellipsoid-shaped voids observed in polymer matrix composites (PMCs), as the former is manufactured via the extrusion technique.

The next step is to characterize the geometry of the embedded ceramic fibers using NURBS functions, as shown in Fig. 4c. The control points and knot vectors of resulting NURBS curves are stored in a virtual shape library. We also extract other information such as average size \( D \) of fibers, their standard deviation \( D_v \) from normal distribution, volume fraction \( V_f \) and two-point correlation function \( S_2(r) \), as well as the variation of voids volume fraction \( V_e \) from imaging data. The RSA algorithm is then employed to construct a raw (simplified) microstructure according to these data with ellipse-shaped inclusions to represent the embedded fibers (Fig. 4d). Diameters of these ellipses are selected such that they circumscribe actual cross sections of the ceramic fibers. In this algorithm, center points of ellipses are randomly distributed in the domain and the inclusions are sequentially created at designated locations only if they do not overlap with an existing inclusion. The periodicity of the microstructure is ensured by creating the

For more details regarding the HIFEM formulation, computational geometry aspects involved in its implementation, and convergence studies refer to Soghrati (2014); Soghrati and Ahmadian (2015); Soghrati and Barrera (2016).
Fig. 4. Schematic of the process of creating virtual RUCs of the Al/Al₂O₃ composite: (a) 3D reconstruction of the MMC microstructure from micro-CT images; (b) composite cross section and the presence of voids; (c) extracting the required data for quantifying the microstructure; (d) raw microstructure created using the RSA algorithm; (e) two sample HIFEM models created by transforming the raw microstructure into more realistic RUCs and incorporating the effect of voids.

Fig. 5. (a) 3D morphology and distribution of voids in the MMC microstructure; (b) Comparison between two-point correlation functions obtained from the imaging data and a virtual RUC with \( l = 30 \) µm.

mirror image of each inclusion that intersect with one of the edges of the domain on the opposite side. To match the two-point correlation function of virtual RUCs with that of the imaging data, a simple approach is implemented: the raw microstructure is created with an approximately 15% higher volume fraction than the target value (\( V_f = 45% \)) and selected fibers are iteratively removed to minimize the least square error between the actual and virtual correlation curves. As shown in Fig. 5b, this simple scheme yields a decent agreement between two-point correlation functions.

To evolve the raw microstructure into realistic HIFEM models of the MMC, we first discretize the RUC domain using a structured mesh, as shown in Fig. 4e. A small portion of this mesh is depicted in the inset of that figure. The NURBS curves representing the pre-existing voids are then virtually embedded in the discretized
domain to create their corresponding children elements in the first level of hierarchy. Next, we employ the subjective mapping between the ellipse-shaped inclusions in the raw microstructure and the NURBS functions characterizing ceramic fibers morphologies to add the fibers to the structured mesh. To accomplish this, we apply a rigid body transformation to control points of each NURBS curve to inscribe that into its corresponding ellipse. Note that, as shown in Fig. 4e, some of the ceramic fibers can overlap with pre-existing voids in the discretized model. However, this is a virtual overlapping between geometric entities defining the voids and the embedded fibers, as only the region outside the fiber is considered as an actual void. Thus, the voids physically do not penetrate the fibers in the resulting HIFEM model. In such cases, the hierarchical enrichment strategy used in this method recursively constructs the enrichment functions to capture weak discontinuities along intersecting materials interfaces.

It must be noted that all the HIFEM simulations presented in the remainder of this manuscript are carried out using structured meshes composed of quadratic elements with the size of \( h = \frac{2}{5} \mu\text{m} \). Each RUC is subjected to a prescribed macroscopic strain, which is incrementally increased at each step to simulate its ductile damage response. Note that this strain-controlled approach can properly handle the transition from the linear elastic (or hardening) to the softening behavior, although very small increments in the macroscopic strain is required in the vicinity of transition points for convergence. To efficiently handle this phenomenon, an adaptive scheme is employed for incrementing the macro-strain: if no convergence is achieved after 10 iterations or if the residuals have an ascending trend in the Newton–Raphson solver, the simulation restarts with half of the current value of the increment in the macro-strain (\( \Delta \varepsilon_\text{M} \)). In contrary, if the convergence is achieved with less than 5 iterations, \( \Delta \varepsilon_\text{M} \) is increased to twice of its current value in the next step. The convergence criterion at each step is to achieve a relative tolerance of \( 10^{-5} \) for the residual force.

Also, for the RUCs studied in this work, the elastic moduli of the ceramic fibers are \( E_c = 300 \text{ GPa} \) and \( \nu_c = 0.24 \), while those of the aluminum matrix are \( E_\text{Al} = 69 \text{ GPa} \) and \( \nu_\text{Al} = 0.3 \). The material parameters needed for simulating the plastic deformation and damage in the aluminum matrix are given in Table 1, which are calibrated with experimental data using the method of variation of plasticity characteristics (Pires et al., 2003).

### 4. Appropriate size of the RUC

In this section, we investigate the optimal size of the periodic RUC for simulating the failure response of the MMC and the impact of the different spatial arrangements of the embedded fibers with similar two-point correlation functions on the mechanical behavior of the RUC. Note that while the assumption of local periodicity in the computational homogenization of heterogeneous materials is violated during damage evolution, the virtual microstructures constructed using the algorithm described in Section 3.2 are statistically equivalent RUCs, for which the macroscopic behavior is equivalent to the average response of the material taking into account local microstructural features (Swaminathan and Ghosh, 2006; Swaminathan et al., 2006). Also, as shown in Nguyen et al. (2008); Terada et al. (2000), the periodic boundary condition is still of the best choices for modeling the microscopic problem provided that the RUC size is sufficiently large.

To determine the appropriate size of the RUC, four periodic domains with lengths \( l = 10, 20, 30, \) and \( 40 \mu\text{m} \) are created using the NURBS-based microstructure characterization algorithm and their failure responses subject to uniaxial macroscopic normal strain in the \( y \) (vertical) direction are simulated using the HIFEM. It must be noted that although based on imaging data such a void-free microstructure does not actually exist, it will be used as a reference solution to quantify the impact of pre-existing voids on the mechanical behavior of the MMC in the following sections. Also, although the two-point correlation functions extracted from the micro-CT images does not necessarily correlate to this hypothetical void-free MMC, we have maintained the same spatial distribution of fibers so that the volume fraction and distribution of voids be the only variable parameters in this study. Fig. 6a illustrates the HIFEM approximation of the macroscopic stress–strain response of the MMC, where the macroscopic stresses are computed according to (6). As shown in that figure, the failure responses of smaller RUCs, i.e., \( l = 10 \) and \( 20 \mu\text{m} \) show a notable size dependence compared to those for the larger RUCs. Based on this study, we choose \( l = 30 \mu\text{m} \) as the appropriate size of the RUC, for which the predicted values of the strength and toughness (absorbed energy)
Fig. 7. (a) Macroscopic stress-strain responses and (b) damage patterns at the failure point in RUCs with \( l = 30 \mu m \) and different spatial distributions of ceramic fibers subjected to uniaxial macroscopic normal strain in the \( y \)-direction.

Fig. 8. Five different distributions of voids in the composite RUC to investigate their impact on the mechanical behavior of the Al/Al\(_2\)O\(_3\) MMC: (a) \( V_v = 0.1\% \); (b) \( V_v = 0.2\% \); (c) \( V_v = 0.4\% \), where \((V)\) indicates the vertical distribution of voids; (d) \( V_v = 0.4\% \), where \((H)\) indicates the horizontal distribution of voids; (e) \( V_v = 0.8\% \).

Fig. 9. Damage evolution in RUCs with (a) no pre-existing voids and (b) \( V_v = 0.4\% \).
are very similar to those of the largest RUC with $l = 40 \, \mu m$. Fig. 6b illustrates damage patterns in these RUCs at the failure point.

To ensure that $l = 30 \, \mu m$ is indeed the appropriate RUC size and does not show size dependency effects, we have also simulated the failure responses of three RUCs with this size but with distinct spatial distributions of embedded fibers. Note that the two-point correlation functions associated with these virtual RUCs are still approximately identical. As expected, Fig. 7a shows that differences between the macroscopic stress-strain responses of the RUCs are negligible. Damage patterns at failure points for two of these RUCs are depicted in Fig. 7b (the third RUC, labeled Microstructure A, is shown in Fig. 6b).

5. Numerical results

In this section, we implement the automated RSA-NURBS-HIFEM framework to investigate the impact of pre-existing voids on the failure response of the MMC subjected to three types of macroscopic loads, applied transverse to the fiber direction: (i) uniaxial normal strain, (ii) equi-biaxial normal strain, and (iii) shear strain. Fig. 8 illustrates five RUCs with $l = 30 \, \mu m$ and identical embedded ceramic fibers but different volume fractions and spatial distributions of pre-existing voids. Note that although volume fractions of pre-existing voids in the RUCs depicted in Figs. 8c and 8d are identical ($V_v = 0.4\%$), they have different spatial distributions (vertical versus horizontal), which can better elucidate the impact of the voids arrangement in the MMC microstructure on its failure response.

5.1. Uniaxial macroscopic normal strain

In this section, we investigate the failure responses of the RUCs with pre-existing voids shown in Fig. 8, as well as that of a perfect RUC with no microstructural defects subject to uniaxial macroscopic normal strain in the $y$-direction. The damage evolution in two RUCs with and without pre-existing voids are depicted in Fig. 9. While in the perfect (void-free) RUC the damage has a relatively uniform distribution within the domain, the pre-existing voids in the RUC shown in Fig. 9b ($V_v = 0.4\%$) serve as primary sites of damage nucleation, which lead to a completely distinct pattern with high concentration of damage in the vicinity of voids. Also, note how the embedded ceramic fibers delay the failure by deviating the damage path, which allows absorbing more energy before failure.

The macroscopic stress-strain responses of the six RUCs studied in this section are illustrated in Fig. 10, which indicates a significant reduction in the strength of the MMC by increasing the voids volume fraction. For example, the presence of voids with the small volume fraction of $V_v = 0.2\%$ leads to a nearly 20% drop in the maximum stress sustained before entering the softening region. This can be attributed to considerably higher stress concentrations in the vicinity of voids, which accelerate the plastic deformation as well as the initiation and propagation of damage in the aluminum matrix. As shown in Fig. 11, this leads to completely different
damage patterns depending on the spatial distribution of voids in the MMC microstructure.

Unlike the MMC strength, its toughness does not directly correlate with the volume fraction of pre-existing voids. For example, the toughness of the RUC with \( V_v = 0.2\% \) is comparable to that of the void-free RUC but significantly higher than the toughness of the RUC with \( V_v = 0.1\% \). A more interesting behavior is observed in the RUCs with 0.4\% void volume fraction, in which the corresponding stress-strain responses are nearly identical until \( \varepsilon_y \approx 0.05 \). However, while the RUC with vertical distribution of voids can sustain the applied load until \( \varepsilon_y \approx 0.15 \), the microstructure with horizontal distribution of voids fails at \( \varepsilon_y \approx 0.06 \), indicating its considerably lower toughness than the former. As shown in Fig. 11, the difference in spatial distributions of voids in these RUCs leads to completely distinct damage patterns at the failure point. Further, the more localized damage pattern in the RUC with \( V_v = 0.4\%^{(H)} \) compared to that with \( V_v = 0.4\%^{(V)} \) indicates the lower energy absorbed by the former before failure. This shows that in addition to the volume fraction of pre-existing voids, their spatial distribution also affects the MMC behavior subjected to uniaxial macroscopic strain.

It must be noted that the peaks and valleys (i.e., alternating softening and hardening regions) observed in the macroscopic stress-strain response of the void-free RUC in Fig. 10 is attributed to the impact of the MMC microstructure on the evolution of the damage. For example, the softening behavior observed after point A is due to the growth of damage in the aluminum matrix until it is being arrested by the ceramic fibers at point B. The MMC can then regain its strength and exhibit a hardening behavior, as the stress is not uniformly distributed within the matrix and therefore some regions of that could show plastic hardening or even elastic behavior until the macroscopic strain reaches point C. It is worth mentioning that the slope of the line segment BC is smaller than the initial slope of the stress-strain curve in the elastic region, indicating that the MMC stiffness is decreased due to a combination of plastic deformation and damage accumulation in some regions of the matrix. Further, note that this alternating
5.2. Equi-biaxial macroscopic normal strain

In this section, we present the results of a study similar to that provided in Section 5.1 to quantify the impact of microstructural voids in the aluminum matrix on the mechanical behavior of the MMC subject to equi-biaxial macroscopic normal strains, applied transverse to the fiber direction. Fig. 12 illustrates damage patterns in the six RUCs, indicating that the damage in the aluminum matrix of the void-free microstructure is highly concentrated along the ceramic fiber/aluminum matrix interfaces. Note that compared to uniaxial macroscopic strain, an equi-biaxial state of stress leads to a lower stress triaxiality in the aluminum matrix away from the embedded fibers; thus it delays the plastic deformation and damage evolution in such regions. However, the high stress concentrations induced in the vicinity of embedded fibers/voids increase the stress triaxiality ratios and therefore serve as primary sites for the damage accumulation in the matrix of the void-free RUC, as illustrated in the top left image in Fig. 12.

The RUCs with microstructural defects depicted in Fig. 12 show that the presence of voids leads to completely different damage patterns than that of the void-free RUC. Compared to the results presented in Fig. 11 (uniaxial macro-strain), the damage induced by equi-biaxial macroscopic strains is more localized. This is attributed to the fact that damage can only initiate either along the ceramic fibers interfaces or pre-existing voids, although the latter demands a lower macroscopic strain for the initiation of damage. Damage patterns in RUCs with higher void volume fractions (bottom row of Fig. 12) are particularly interesting, as they are concentrated on imaginary lines that connect pre-existing voids to one another. It is also worthwhile to more meticulously study the damage developed in RUCs with $V_v = 0.4^{(V)}$ and $V_v = 0.4^{(H)}$, where despite the similarity of void volume fractions and symmetry of the loading in the $x$ and $y$ directions, two distinct patterns of damage and thus failure modes are observable. This re-emphasizes the notable impact of the spatial distribution of voids and not merely their volume fraction on the mechanical behavior of this MMC, which also shows the difficulty in predicting its failure response due to the uncertainty in the distribution of microscopic defects at different macroscopic locations.

To shed more light on the uncertainty caused by microstructural defects on the failure response of the Al/Al$_2$O$_3$ composite, the stress-strain behaviors of all six RUCs are presented in Fig. 13. Due to the effect of the lower stress triaxiality in delaying the damage initiation in the aluminum matrix, the void-free RUC shows a higher strength than when subjected to uniaxial macroscopic strain. The stress-strain responses of the other five RUCs show that pre-existing voids have a considerable effect on reducing both the strength and toughness of the MMC. Similar to the results presented for the uniaxial loading (Fig. 10), while the higher the volume fraction of voids the lower the strength, no clear relationship can be established between the voids volume fraction and the local toughness of the MMC.

5.3. Macroscopic shear strain

In contrary to the studies presented in Sections 5.1 and 5.2, which show that pre-existing voids considerably deteriorate the mechanical strength of the MMC when subjected to macroscopic normal strains, simulating the failure response of this material under shear loading reveals a different behavior. The stress-strain responses of the six RUCs subjected to macroscopic shear strain, applied transverse to the fiber direction, are depicted in Fig. 14. These results indicate that no meaningful relation exists between the strength and toughness of the MMC with the volume fraction and spatial distribution of voids in this case.
Fig. 15 illustrates that damage patterns at the failure point in the RUCs subjected to macroscopic shear strain, which unlike the case scenarios depicted in Figs. 11 and 12, shows slight differences in the damage pattern in the vicinity of voids. The similarity of these damage patterns suggests that when subjected to shear loading, voids are not the primary driving force for the initiation and propagation of damage in the MMC microstructure. This study indicates that the type of loading is also a major factor in determining how pre-existing voids affect the strength and toughness of the MMC.

6. Conclusion

An automated computational framework was employed to investigate the impact of pre-existing voids on the failure response of a ceramic fiber reinforced aluminum matrix composite subject to loadings applied in transverse to the fiber direction. A strain-driven computational homogenization model relying on the Lemaître elasto-plastic damage model was implemented to simulate the initiation and evolution of damage in the aluminum matrix. To automate aspects of the modeling process, a new NURBS-based microstructure quantification algorithm was employed to generate virtual microstructural models of the composite based on micro-CT imaging data. The hierarchical interface-enriched FEM was also used to perform mesh-independent damage simulations. Six virtual microstructural models with varying volume fractions and size/spatial distributions of voids subject to three types of macroscopic loads were analyzed. Main outcomes of this study can be summarized as follows: (i) When subjected to macroscopic normal strains, even a very small volume fraction of voids considerably deteriorates the composite strength. (ii) While the reduction in strength is directly proportional to the volume fraction of voids, variations of the toughness is highly dependent on the spatial distribution of voids, and does not necessarily deteriorate due to the presence of voids. (iii) When subjected to macroscopic shear strains, small volume fractions of pre-existing voids in the aluminum matrix does not have a notable impact on the failure response.

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