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

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**A B S T R A C T**

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.

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

$$\mathbf{u}(\mathbf{x}_m, \mathbf{x}_n) = \mathbf{u}_m(\mathbf{x}_m) + \mathbf{u}_n(\mathbf{x}_n).$$

The strong form of the governing equations describing the response of $\Theta$ subject to macroscopic strain $\varepsilon_m$ can be expressed as:

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Find the microscopic displacement filed \( u_m \) such that

\[
\begin{align*}
\nabla \sigma_m &= 0 \quad \text{in } \Theta \\
\sigma_m &= C : \varepsilon_m^e \quad \text{in } \Theta \\
\varepsilon_m^e &= \frac{1}{2} (\nabla u_m + \nabla u_m^T) \quad \text{in } \Theta.
\end{align*}
\]

where \( \sigma_m \) is the microscopic Cauchy stress tensor, \( C \) is the fourth-order elasticity tensor, and \( \varepsilon_m^e \) is the microscopic elastic strain tensor. The weak form of (2) can be written as: Find \( u_m \in V := \{ u_m : \Theta \to \mathbb{R}^2 \} \) such that

\[
\frac{1}{|\Theta|} \int_{\Theta} \sigma_m : \nabla u_m \, d\Theta = 0,
\]

where \(|\Theta|\) is the measure (area) of \( \Theta \). The Hill–Mandel micro-homogeneity principle (Hill, 1985) can be employed to relate the potential energy \( \Phi_M \) at a macroscopic point to the average potential energy density \( \Phi_m \) at its corresponding microscopic RVE as

\[
\inf_{u_m} \Phi_M(\varepsilon_m) = \inf_{\varepsilon_m} \frac{1}{|\Theta|} \int_{\Theta} \Phi_m(\varepsilon_m + \varepsilon_m) \, d\Theta.
\]

Applying standard variational principles to (4) and noting that the microscopic displacement field \( u_m \) makes no contribution to the average microstructural energy (Kouznetsova et al., 2002), \( \sigma_M \) can be computed as (Soghrati and Liang, 2016)

\[
\sigma_M = \frac{1}{|\Omega|} \int_{\Omega} \sigma_m \, d\Omega.
\]

2.2. Continuum brittle damage model for the SiC particles

In order to simulate the initiation and evolution of damage in the SiC particles, we adopt an isotropic continuum brittle damage model similar to that described in Matouš et al. (2008). In this model, a scalar parameter \( \omega \) ranging from 0 (virgin material) to 1 (fully damaged) is employed to incorporate the effect of damage on the energy potential \( \Phi_m(\varepsilon_m) \) at the macroscale as

\[
\Phi_m(\varepsilon_m, \omega) = (1 - \omega) \Phi_m(\varepsilon_m).
\]

The following function is then implemented to describe the onset of damage in the particles

\[
g(\Phi_m(\varepsilon_m), \chi^2) = G(\Phi_m(\varepsilon_m) - \chi^2) \leq 0, \quad t \in \mathbb{R}^+,
\]

where \( \chi^2 \) is an internal state variable and \( G(\Phi_m(\varepsilon_m)) \) is a Weibull distribution function expressed as

\[
G(\Phi_m(\varepsilon_m)) = 1 - \exp\left(\Phi_m(\varepsilon_m)/\Phi_m^{p_1}\right)^{p_2}.
\]

In (10), \( \Phi_m^{p_1} \) is the energy threshold corresponding to the initiation of damage, while the scalar parameters \( p_1 \) and \( p_2 \) determine the shape of the damage surface. The rate of damage progression \( \dot{\omega} \) in the material is given by

\[
\dot{\omega} = \mu \frac{\partial g(\Phi_m(\varepsilon_m), \chi^2)}{\partial \Phi_m(\varepsilon_m)} = \mu \frac{\partial G(\Phi_m(\varepsilon_m))}{\partial \Phi_m(\varepsilon_m)},
\]

where \( \mu \) is the damage viscosity coefficient. It must be noted that the viscous regularization scheme presented in Simo and Ju (1987) is combined with (11) to mitigate the mesh dependency effects associated with the use of this continuum damage model by regularizing the damage localization.

2.3. Plane stress-projected plastic model for the Al matrix

In order to simulate the plastic behavior of the Al matrix, we implement a plane stress-projected von Mises elastoplastic model with isotropic hardening, as originally described in Simo and Taylor (1986). Using a plane stress model to simulate the MMC mechanical behavior and in order to satisfy the constraint of zero out-of-plane stresses, the yield function \( \Psi \) is defined as

\[
\Psi = \frac{1}{2} \sigma_m^T \mathbf{P} \sigma_m - \frac{1}{3} \kappa^2 \hat{\varepsilon}^2.
\]

In the equation above, \( \kappa(\hat{\varepsilon}) \) describes the material hardening in terms of the equivalent plastic strain \( \hat{\varepsilon}^p \) and \( \mathbf{P} \) is a transformation matrix used for evaluating the deviatoric stress tensor \( \mathbf{s} \). The plastic flow rule and the hardening variable \( \hat{\varepsilon}^p \) evolution are expressed as

\[
\hat{\varepsilon}^p_m = \gamma \mathbf{P} \sigma_m, \quad \hat{\varepsilon}^p = \gamma \sqrt{3} \sigma_m^T \mathbf{P} \sigma_m.
\]

where \( \gamma \) is the plastic Lagrange multiplier.

For the numerical implementation of this plasticity model, we implement a strain-driven implicit integration algorithm. In this approach, an elastic predictor with a given in-plane incremental strain \( \Delta \varepsilon_m \) at time step \( t_n \) is employed to check the plastic admissibility given in (12). If the elastic trial state is not admissible, we use the return-mapping algorithm to solve the following nonlinear equation

\[
\Psi(\Delta \gamma) \equiv \frac{1}{2} \xi(\Delta \gamma) - \frac{1}{3} \kappa \left[ \hat{\varepsilon}^p + \Delta \gamma \sqrt{3} \xi(\Delta \gamma) \right] = 0.
\]

where \( \xi(\Delta \gamma) \) is the nonlinear plane stress-projected return-mapping equation. The elastoplastic consistent tangent moduli evaluated based on (14) are then employed to improve the convergence rate at each step.

It must be noted that the solid state powder metallurgy, which is often used for manufacturing Al/SiC MMCs, facilitates strong interface bonding between particles and the matrix, which can
be modeled as a perfectly bonded interface (Chawla et al., 1998; Williams et al., 2002). Therefore, in this work, we do not use cohesive elements to simulate the debonding along particle/matrix interfaces.

3. Automated construction of virtual microstructures

In this section, we present a new algorithm for the automated construction of realistic periodic RVEs of particulate MMCs with the desired morphology, volume fraction, size distribution, and spatial arrangement of embedded particles. The aim of the proposed approach is to reduce the algorithmic complexity and computational cost associated with the reconstruction of virtual RVEs of such composite materials, while maintaining realistic microstructural features. Fig. 1 schematically shows the stepwise reconstruction of an Al/SiC MMC microstructure using this algorithm. Next, we describe each step in more details.

- Step 1: Periodic Voronoi decomposition

As shown in Fig. 1a, the first step of the reconstruction of the MMC microstructure is to tessellate the RVE domain using the Voronoi decomposition algorithm. The Voronoi tessellation of a two-dimensional Euclidean space is described as (Benedetti and Aliabadi, 2013)

\[ C_i \subseteq \{ x \in \mathbb{R}^2 \mid d(x, s_i) < d(x, s_j) \forall j \neq i \} \]

where \( C_i \) denotes a collection of Voronoi cells (partitions), \( s_i \) is the seed point corresponding to \( C_i \), and \( d(x, s_i) \) is the Euclidean distance between point \( x \) and \( s_i \). The density of these randomly distributed source points is determined such that assigning a particle with an average size to each seed point yields a volume fraction that is at least twice of the target volume fraction of the particles. Also, since we aim to build a periodic RVE, eight copies of the seed points are created along the four edges and four corners of the domain to form a \( 3 \times 3 \) grid of identical sets of source points. The central set and the seed points created adjacent to them by these copies are then utilized for the construction of Voronoi cells that are periodic along the domain boundaries.

- Step 2: Centroidal Voronoi tessellation

Due to the random distribution of Voronoi seed points and thus the randomness of the shape of corresponding cells, transforming each cell into an SiC particle does not yield the desired shape, size distribution, and spatial arrangement. To provide a more uniform distribution of Voronoi cells, we implement the Centroidal Voronoi Tessellation (CVT) (Lloyd, 1982) algorithm to create cells with similar sizes, as depicted in Fig. 1b. To achieve this, the CVT employs an iterative algorithm, in which seed points are relocated to the centroids of their corresponding Voronoi cells in each iteration to provide a uniform distribution of seed points in the domain.

- Step 3: Erosion and random movement

In order to replicate the desired size distribution and aspect ratios of particles, we apply a modified version of the erosion algorithm (Fritzen and Höhle, 2011) to the Voronoi cells constructed using the CVT algorithm, as shown in Fig. 1c. In this algorithm, a randomly oriented local coordinate system \((x_i, y_i)\) is assigned to each cell. The cells are then shrunken in the \( y_i \) direction according to a probability density function representing the aspect ratios of particles, which can be extracted from imaging data. The cells are then uniformly eroded such that the areas (\( A \)) of resulting polygons match another probability density function representing the particles size distribution. Here, the aspect ratio (\( AR \)) of particles is defined as

\[ AR = \frac{4d_{\text{max}}^2}{\pi A} \]

where \( d_{\text{max}} \) is maximum distance between any two points on the surface of the particle.
To maintain a random distance between the particles after eroding the cells, each polygon is then relocated randomly within the walls of its original Voronoi cell. The completion of this step yields a microstructure template with at least twice higher volume fraction than the target value. In this work, the size and aspect ratio distributions of the SiC particles in the MMC microstructures are described using log-normal functions. For each parameter $\alpha$, the log-normal probability function can be written as (Borbel et al., 2004)

$$f(\alpha) = \frac{1}{\sqrt{2\pi} S} \exp\left(-\frac{(\ln \alpha - N)^2}{2S^2}\right).$$

(17)

where $N$ is the mean value and $S$ is the standard deviation. Fig. 2 shows the probability density functions describing the size ($N_i = 0.08$, $S_i = 0.12$) and aspect ratio ($N_\alpha = 0.99$, $S_\alpha = 0.3$) distributions of the SiC particles used in this work, which are extracted from the imaging data presented in Brechet et al. (1991).

- Step 4: Sequential elimination of particles

The next step is to sequentially remove the particles from the microstructure template constructed in the previous step until the remaining particles yield the target volume fraction and spatial arrangement (Fig. 1d). In this work, the spatial arrangement of the SiC particles is characterized using a nearest neighbor distance probability function $F(R)$. This function is defined such that $F(R)\,dR$ is the probability that the centroid of a particle is located between distances $R$ and $R + dR$ from its nearest neighbor particle (Bansal and Ardell, 1972). Similar to the size and aspect ratio distributions, we use a log-normal probability function for $F(R)$ with the standard deviation of $S_d = 0.2$. Three different mean values are considered for this function to characterize the effect of the spatial arrangement of the SiC particles on the mechanical behavior of the MMC: $N_d = 0.36$ (uniform distribution), $N_d = 0.20$ (slightly clustered), and $N_d = 0.13$ (highly clustered). Further, we aim to quantify the impact of three particles volume fractions ($V_p = 10\%$, $20\%$, and $30\%$) on the stiffness, strength, and toughness of this particulate composite.

In each step of the proposed sequential elimination algorithm, we only select one particle to remove from the RVE such that the discrepancies between the target statistical descriptors (size, aspect ratio, and nearest neighbor distance distribution functions) and those of the virtual microstructure are minimized. The discrepancy error function $E_d$ to be minimized is defined as the weighted sum of squared differences between the areas under the target and simulated correlation functions ($L_2$-norm of the error), which can be written as

$$E_d = \sum_{i=1}^{n_p} \sum_{j=1}^{3} w_j \| f_j(i) - \tilde{f}_j(i) \|_2.$$  

(18)

In this equation, $\| \cdot \|_2$ is the norm of the function, $n_p$ is the number of particles, and $f_j$ is the statistical descriptor, in which $j$ refers to the size ($j = 1$), aspect ratio ($j = 2$), and nearest neighbor distance ($j = 3$) distribution functions. Also, $w_j$ is the weight for each descriptor and $\tilde{f}_j$ is the target correlation function. Here, similar to Balzani et al. (2014) and Olchawa and Piasecki (2015), we performed a parametric study to select $w_1 = w_2 = 1$ and $w_3 = 4$ for constructing the final virtual microstructures. Fig. 3 compares the target nearest neighbor distance functions with those generated using this sequential elimination algorithm for different spatial arrangements of the SiC particles in three $25 \mu m \times 25 \mu m$ virtual RVEs with $V_p = 30\%$.

- Step 5: NURBS parameterization

The completion of the previous step yields a raw microstructure, which attains all the desired microstructural features except for the realistic morphology of the particles. To resolve this issue, each polygonal-shaped particle is substituted with a Non-Uniform Rational B-Splines (NURBS) (Piegl and Tiller, 2012) parameterization of its morphology, as shown in Fig. 1e. A NURBS curve $C(u)$ is a function of the parametric coordinate $u$, which is composed of $n$ B-splines of order $p$, $M^p_i(u)$. $C(u)$ is evaluated by interpolating the B-spline functions over a set of $n$ control points with physical coordinates $x_i$ and given weights $w_i$, i.e.,

$$C(u) = \sum_{i=1}^{n} x_i w_i M^p_i(u).$$

(19)

A set of $n + p + 1$ breakpoints $U = \{u_1, u_2, u_3, \ldots, u_{n+p+1}\}$ (knot vector) is employed to divide the parametric space $u$ into smaller intervals. $C(u)$ is a $C^0$-continuous function, which is not differentiable at the breakpoints.

To build the final microstructure, we first create a set of control points at the corners and midpoints of edges of each polygon and generate an initial NURBS curve to more realistically capture the SiC particles morphologies. As shown in Fig. 1e, some of the control points are subsequently moved inward along the direction...
of the normal vector to edges of the Voronoi cells to simulate the concave shape of particles, which is observable in the microstructure of some Al/SiC particulate MMCs (Brechet et al., 1991). The probability of the inward movement of a control point can be determined based on the percentage of concave particles in the imaging data. It must be noted that the difference between the areas of shrunk Voronoi cells and that the NURBS curves are on average less than 1%. Therefore, to precisely replicate the target volume fraction in the virtual microstructure, we create the raw microstructure (Step 4) with a volume fraction that is 1% higher than the target value. After replacing the polygon-shaped particles with NURBS curves representing the actual shapes of particles, the volume fraction of the final virtual microstructure will nearly be identical to the desired value. Fig. 4 illustrates six 25 μm × 25 μm periodic microstructures of the Al/SiC MMC with varying volume fractions and spatial arrangements of the embedded particles generated through this five-step algorithm.

4. CISAMR: Non-iterative mesh generation algorithm

To study the mechanical behavior of the Al/SiC MMC, we must convert the virtual RVEs created using the CVT-NURBS reconstruction algorithm into appropriate FE models. In order to automate this process, we implement the Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) technique introduced by Soghrati et al. (2017). As shown in Fig. 5, the CISAMR transforms a simple structured grid into a hybrid conforming mesh composed of rectangular and triangular elements with proper aspect ratios. One of the key advantages of this method compared to other sophisticated mesh generation algorithms such as Quadtree based techniques (Yerry and Shephard, 1984; Baehmann et al., 1987) is the non-iterative approach used for the construction of the mesh, which highly facilitates its implementation and eliminates the need for smoothing algorithms to improve the mesh quality. For completeness, in this section we provide a brief overview of
the CISAMR algorithm, together with discussing the additional considerations required for creating periodic FE models of the MMC microstructure.

- **Step 1: h-adaptivity**

  As the first step, we employ a customized Structured Adaptive Mesh Refinement (SAMR) algorithm to locally refine the background mesh in the vicinity of materials interfaces, as shown in Fig. 5a. In reducing the geometric discretization error, this SAMR phase enables a more accurate approximation of stress concentrations along the Al/SiC interfaces. In this algorithm, at each level of refinement, we identify the background elements intersecting with materials interfaces and subdivide them into four sub-elements. We then refine neighboring elements sharing each node of a nonconforming element provided that the node is located in a different material phase compared to the midpoint of one of the edges connected to that. A detailed discussion is provided in Soghrati et al. (2017) on the SAMR constraints that must be satisfied to ensure the sufficient number of refinement levels for regions that particles are close to one another or in the vicinity of domain boundaries. Here, we consider an additional constraint to preserve the periodicity of the discretized FE model of the MMC microstructure. For this purpose, if a background element located along one of the domain boundaries is subjected to refinement, we locate the element with either the same x or y coordinate on the parallel edge and apply the same level of refinement to that. Satisfying this constraint ensures that regardless of the complexity of the microstructure, identical nodes are created on two parallel edges of the domain. As noted previously, the periodic BC can then be applied to these nodes by assigning the same microscopic displacement to each pair of periodic nodes, which is equivalent to assigning similar equation numbers for assembling the stiffness matrix.

- **Step 2: r-adaptivity**

  A non-iterative r-adaptivity algorithm is then applied to relocate selected nodes of the background elements cut by Al/SiC interfaces to construct a deformed mesh similar to that depicted in Fig. 5b. A key advantage of this algorithm is that the new location of each node is independent of the relative distances between its adjacent nodes and other materials interfaces. Assuming that the distance between a mesh node and the intersection point of the materials interface with one of the edges with length \( h \) connected to that node, the new location of this node is determined according to the following algorithm:

  1. If one of the edges connected to that node is cut by the interface: (a) If \( d \geq 0.5h \), the node remains intact. (b) If \( d < 0.5h \), the node moves to the edge/interface intersection point.

  2. If both edges connected to that node are cut by the interface: (a) If \( d_1 \geq 0.5h_1 \) and \( d_2 \geq 0.5h_2 \), the node remains intact. (b) If \( d_1 < 0.5h_1 \) and \( d_2 \geq 0.5h_2 \), the node moves to the intersection point at distance \( d_1 \). (c) If \( d_1 < 0.5h_1 \) and \( d_2 < 0.5h_2 \), the node moves to the intersection point at distance \( d_1 \) and the intersection point at distance \( d_2 \) is discarded.

- **Step 3: Sub-triangulation**

  Finally, the elements deformed during the r-adaptivity process and those with hanging nodes on their edges due to the SAMR of neighboring elements are sub-triangulated to create a conforming mesh (Fig. 5c). The sub-triangulation process for the latter case is straightforward and could result in the construction of 3 to 8 triangular sub-elements, depending on the number of edges with hanging nodes (between 1 and 4). For the former case, to ensure that aspect ratios of resulting sub-elements are lower than three, we use the following rules sub-triangulating a nonconforming element:

  1. If the element is not cut by the interface along the diagonal emanating from its smallest angle \( \theta_{\text{min}} \), always cut the element along the diagonal emanating from its largest angle to create two conforming sub-triangles.

  2. Otherwise: (a) if \( \theta_{\text{min}} > 60^\circ \), sub-triangulate by cutting along \( \theta_{\text{min}} \); (b) if \( \theta_{\text{min}} < 60^\circ \), subdivide by cutting along both diagonals, which results in the creation of four conforming sub-triangles.

5. **Linking microstructure to the mechanical behavior**

In this section, we employ the CVT-NURBS-CISAMR framework to characterize the effects of volume fraction and spatial arrangement of the SiC particles on the stiffness, strength, and toughness of the MMC. The mechanical properties of the Al 2024-T6 alloy matrix are \( E_A = 75.47 \) GPa, \( \nu_A = 0.33 \), and \( E_p = 387.4(0.0054 + \nu_p)^{0.163} \) MPa, while those of the SiC particles are \( E_S = 410 \) GPa and \( \nu_S = 0.19 \) (Brechet et al., 1991; Geni and Kikuchi, 1998). Also, the
required parameters for simulating brittle damage in the SiC particles are $\Phi^\text{mm} = 0.1$ MPa, $p_1 = 50$, and $p_2 = 0.3$, which are calibrated based on the data provided in Llorca et al. (1993). As suggested in Mosby and Matouš (2015), a viscous parameter of 100 s$^{-1}$ is employed to reduce the mesh dependency effect associated with the use of this continuum damage model. As noted previously, we study the effect of three different volume fractions ($V_p = 10\%$, 20\%, 30\%) and spatial arrangements ($N_d = 0.36$, 0.2, 0.13) on the mechanical behavior of this MMC.

5.1. Appropriate size of the statistical RVE

Before investigating the impact of microstructure on the MMC’s structural integrity, we must determine an appropriate size of the microstructural model that can serve as an RVE for this composite material. To achieve this, we implemented the CVT-NURBS-CISAMR to simulate the micromechanical behavior of multiple periodic microstructural models with lengths $l = 15\mu$m, 25\mu$m, and 50\mu$m subject to a macroscopic uni-axial tensile strain in the y-direction. For each length, nine virtual microstructures corresponding to different permutations of $V_p$ and $N_d$ were created and analyzed. Fig. 6 shows the resulting macroscopic stress–strain responses of the models with $V_p = 20\%$ and 30\% and highly clustered spatial arrangement of the SiC particles ($N_d = 0.13$). These figures indicate that the mechanical responses of the smallest microstructural model ($l = 15\mu$m) exhibit a notable size dependence effect compared to those of the larger models. We select $l = 25\mu$m as the appropriate size for the RVE, as the predicted values of the strength and toughness (absorbed energy) are similar to those of the microstructural model with $l = 50\mu$m. It is worth mentioning that a similar behavior is observed in the results corresponding to periodic microstructures with other values of $V_p$ and $N_d$ that are not presented in Fig. 6.

To ensure that $l = 25\mu$m is indeed the appropriate size of the RVE and does not show size dependency effects, we have also studied the micromechanical behaviors of three virtual RVEs of MMCs with volume fractions $V_p = 20\%$ and 30\%. As shown in Fig. 7, for $V_p = 30\%$, the RVEs have distinct microstructures but similar spatial arrangements of the embedded SiC particles ($N_d = 0.13$). Fig. 8 illustrates the macroscopic stress–strain responses of the RVEs, obtained from FE simulations relying on conforming meshes generated using CIASMR, which shows negligible differences in the behavior of microstructures with similar volume fractions and spatial arrangements. This study verifies that $l = 25\mu$m is the appropriate size of the RVE for this MMC subject to uniaxial loadings.

5.2. Effect of the particles spatial arrangement

Fig. 9 shows the variation of the homogenized stress–strain responses of RVEs with different spatial arrangements of SiC particles subject to macroscopic normal and shear strains. Similar to the results presented in Segurado and Llorca (2006) and Castaneda and Suquet (1997), the current study shows that particles clustering has a negligible impact on the stiffness of the MMC. Secondly, the mechanical response is not affected by the spatial arrangement of the particles in the Al matrix for a considerable portion of the plastic region past the yield point (up to a macroscopic strain of $\epsilon_y \approx 0.075$). After this point, in particular when the RVE is subjected to a macroscopic shear strain, the spatial arrangement of particles has a more notable impact on the mechanical behavior. In this case, although the particle clustering only slightly deteriorates the strength ($\approx 1.5\%$, Fig. 9d), it can lead to approximately...
Fig. 8. Effect of varying microstructures with similar statistical spatial arrangements of the embedded particles ($N_d = 0.13$) on the macroscopic stress–strain responses of MMCs with $l = 25$ μm and subject to a macroscopic normal strain: (a) $V_p = 20\%$; (b) $V_p = 30\%$.

Fig. 9. Effect of the spatial arrangement of SiC particles on the macroscopic stress–strain responses of RVEs with following volume fractions and macroscopic loadings: (a) $V_p = 10\%$, normal strain; (b) $V_p = 10\%$, shear strain; (c) $V_p = 20\%$, normal strain; (d) $V_p = 20\%$, shear strain; (e) $V_p = 30\%$, normal strain; (f) $V_p = 30\%$, shear strain.

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7% reduction in toughness of the MMC (Fig. 9f), which is consistent with the results obtained using the nonlinear homogenization methods in Castaneda and Suquet (1997) and Michel et al. (2001).

The difference in the macroscopic stress–strain responses of RVEs with varying spatial arrangements of the SiC particles, as seen in Fig. 9, is mainly attributed to the accumulation of damage in the particles. Fig. 10 illustrates the von Mises stress fields in the Al matrix at the last step of the simulation, as well as the damage parameter in the embedded SiC particles, in three RVEs with \( V_p = 30\% \) and different levels of particles clustering subject to a macroscopic shear strain. A larger percentage of fully damaged particles are observed in the RVEs with the highest level of clustering in Figs. 10(d–f), which can be attributed to higher stress concentrations in regions with high particle clustering. This accumulation of damage explains the higher rate of softening and therefore the lower toughness associated with such microstructures. However, the strength of the MMC is largely unaffected by the spatial arrangement of particles due to the redistribution of the stresses in the Al matrix.

It is worth mentioning that according to the nearest-neighbor distance functions used in this study (see Fig. 3), the minimum spacing between particles in RVEs with uniform particles distribution is considerably larger than those with slightly and highly clustered distributions. However, this value is approximately identical for the latter two cases. According to Figs. 10(a–c), regions with minimum particle spacing correspond to the highest von Mises stress concentrations in the Al matrix, which lead to the plastic deformation and softening behavior of the MMC. Thus, the nearest-neighbor distance functions used for the construction of the virtual RVEs explain the similarity of the stress–strain responses of RVEs with slightly and highly clustered particles and their considerable difference with the behavior of RVEs with uniformly distributed particles (Fig. 9).

### 5.3. Effect of the particles volume fraction

Fig. 11 illustrates the effect of the volume fraction of particles on the macroscopic stress–strain responses of highly clustered \( N_d = 0.13 \) composite RVEs subject to macroscopic normal and shear strains. As shown in Section 5.2, the effect of the spatial arrangement of particles on the linear elastic response of the MMC is negligible. Table 1 presents the predicted values for the elastic moduli using the CVT-NURBS-CISAMR algorithm (i.e., slope of the linear portion of the macroscopic stress–strain curve) for varying volume fractions of particles. Similar to Saheli et al. (2008), we validate our results by comparing the effective moduli with the homogenized values evaluated using the following micromechanical models: the rules of mixture bounds (Voigt, 1889; Reuss, 1929).

![Fig. 10. (a–c) von Mises stress in the Al matrix and (d–f) damage parameter in the SiC particles of RVEs with \( V_p = 30\% \) and different spatial arrangements of particles (left: uniform distribution; middle: slightly clustered; right: highly clustered) subject to a macroscopic shear strain.](image)

<table>
<thead>
<tr>
<th>Model</th>
<th>( V_p = 10% )</th>
<th>( V_p = 20% )</th>
<th>( V_p = 30% )</th>
</tr>
</thead>
<tbody>
<tr>
<td>FE simulation</td>
<td>84.9</td>
<td>95.8</td>
<td>109.3</td>
</tr>
<tr>
<td>Rules of mixture</td>
<td>82.2–110.5</td>
<td>89.8–144.8</td>
<td>100.0–178.5</td>
</tr>
<tr>
<td>HSS</td>
<td>870–970</td>
<td>100.4–120.2</td>
<td>115.0–145.3</td>
</tr>
<tr>
<td>Mori-Tanaka</td>
<td>88.3</td>
<td>100.3</td>
<td>111.1</td>
</tr>
<tr>
<td>Eshelby</td>
<td>86.2</td>
<td>97.0</td>
<td>107.6</td>
</tr>
<tr>
<td>Self-consistent</td>
<td>85.2</td>
<td>97.1</td>
<td>112.2</td>
</tr>
</tbody>
</table>

Table 1 Elastic moduli (GPa) evaluated based on the CVT-NURBS-CISAMR simulations and their comparison with the values predicted using different analytical micromechanical models for RVEs with different volume fractions of the SiC particles.
Hashin–Shtrikman bounds (Hashin and Shtrikman, 1963) (denoted as HSB), Mori–Tanaka method (Mori and Tanaka, 1973; Benveniste, 1987), Eshelby model (Eshelby, 1957), and self-consistent estimate (Hill, 1965). While this comparison verifies the results obtained from the FE simulations, it also indicates that simpler micromechanical models can accurately predict the elastic moduli of the MMC without taking into account the effect of the shape, size distribution, and spatial arrangement of particles. However, as the Al matrix enters the plastic region and the damage is developed in SiC particles, such microstructural features play an important role in the mechanical behavior of this composite material, which cannot be predicted using an analytical micromechanical model.

Fig. 11a shows the macroscopic stress–strain responses corresponding to different volume fractions of SiC particles in highly clustered RVEs subjected to a macroscopic tensile strain. It is observed that although increasing the volume fraction only slightly increases the strength of the MMC (≈1%), it has a considerable negative impact on its toughness. Fig. 12 illustrates the von Mises stress fields in these RVEs, together with the damage patterns in the particles. Analyzing the impact of the volume fraction on the
strength and toughness of the MMC under a macroscopic shear loading reveals a more interesting trend, as increasing the volume fraction significantly deteriorates both the strength and the toughness (Fig. 11b). Moreover, unlike the RVEs subjected to a macroscopic tensile strain, a considerable amount of damage is developed in the SiC particles before the onset of plastic deformation in the AI matrix under this type of loading. These damaged particles behave similarly to voids within the MMC microstructure when additional macroscopic shear strain is applied, which contributes to significant reductions in both its strength and toughness by increasing the volume fraction. Hence, embedding particles with a higher damage threshold can potentially obviate this shortcoming and lead to an improved strength under shear loading. Note that the main objectives of incorporating brittle SiC particles in such MMCs are often to provide superior thermal performance and prevent resonance vibration rather than improving the mechanical behavior (Cui et al., 2008).

6. Conclusions

An integrated computational framework was presented for creating realistic RVEs of Al/SiC particulate composites, and subsequently generating high quality conforming FE meshes for investigating the impact of microstructure on their mechanical behavior. The proposed methodology relies on a new microstructure reconstruction algorithm combining the CVT, erosion and random movement of Voronoi cells, and sequential elimination of the resulting particles to simulate the desired size distribution, volume fraction, and spatial arrangement of particles. The realistic morphology of the particles is replicated by employing the NURBS parameterization of their shapes. The CISAMR technique was then implemented to automatically create high fidelity FE models of the virtual microstructures by transforming a structured grid into an appropriate conforming mesh using a non-iterative algorithm.

After characterizing the appropriate size of the RVE, nine virtual microstructural models with varying volume fractions and spatial arrangements of particles subject to macroscopic normal and shear strains were analyzed. A brittle damage model was adopted to simulate the fracture of SiC particles, together with a plane stress-projected plasticity model for simulating the nonlinear mechanical behavior of the AI matrix. Main observations of this study can be summarized as follows: (i) The particles clustering reduces the toughness but has a negligible impact on the stiffness and strength of the composite; (ii) When subjected to a macroscopic tensile strain, increasing the volume fraction of particles slightly improves the strength but considerably deteriorates the toughness; (iii) When subjected to macroscopic shear strain, increasing the volume fraction of particles significantly deteriorates both the toughness and the strength of the MMC.

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