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THE VORONOI CELL FINITE ELEMENT METHOD FOR RESPONSE AND DAMAGE ANALYSIS OF ARBITRARY HETEROGENEOUS MEDIA

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of The Ohio State University

By

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ABSTRACT

In this dissertation, the Voronoi Cell Finite Element Method (VCFEM) is innovated for material/failure characterization of ductile arbitrary heterogeneous media. The finite element mesh emerges naturally through the Dirichlet tessellation of the microstructure as a network of multisided polygons, with each polygon containing one heterogeneity at most. The resulting Voronoi polygons are treated as finite elements without any further discretization of the microstructural domain. A computational scheme is formulated through the assumed stress hybrid variational principle to solve for the microstructural deformations under the application of macroscopic loading. The two field variational principle automatically allows for multi sided finite elements, through independent assumptions on the deformations on the element boundary and stresses within the element. Constitutive response of the matrix and heterogeneity phases of the microstructure are modeled as rate-independent elastic-plastic $J_2$ materials and the kinematics is analyzed within the framework of 2-d small deformations of the constituents. Damage in the microstructure is initiated by cracking/splitting of the particles triggered through a maximum principle stress theory or Rankine criterion. This model allows for progressive failure of the material without any user interference. Numerical validation of the VCFEM is established through comparison with analytical and traditional finite element methods. Applicability of the current
scheme to model damage in arbitrary media is demonstrated for computer generated/actual microstructures. Effect of stereographic features such as shape, size and distribution of heterogeneities on damage evolution in random microstructures are also discussed. Statistical representations, that correlate microstructural morphology with material failure, are used to derive the required length scales for the microstructural problem.
To my Mother and Father
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CHAPTER 1

INTRODUCTION

1.1 Motivation

The last two decades have seen a surge in the utilization of functionally superior heterogeneous materials for engineering applications. Important classes of materials among them are metal/alloy systems with microscopic precipitates and pores, and composites containing a dispersion of fibers, whiskers or particulates in the matrix. This has necessitated the development of robust analytical/numerical models for predicting effective material properties and evolving state variables in the microstructure. Design of such materials require accurate simulation of the deformation processes in the microstructure in order to predict overall properties of these materials during linear and non-linear stages of the external loading process. Of particular interest are the effects of microstructural morphology such as shapes, sizes, orientations and location of second phase inclusions on deformation characteristics, like plastic strains and stresses, and developments of material properties like strain hardening.

A large number of analytical micromechanical models have been proposed for predicting effective constitutive response at the macroscopic level. Notable among various analytical micromechanical models for brittle materials are those based on
variational approach using extremum principles [1], probabilistic approaches [2], self-consistent schemes [3, 4] and the generalized self consistent models [5]. Though analytical micro-mechanical models are reasonably effective in predicting equivalent material properties for simple geometries and low second phase volume fractions, arbitrary distribution of shapes, sizes and location in real materials, cannot be deterministically treated. Constitutive response of the constituent phases are also restricted, and predictions with large property mismatches are not reliable. Further, relatively fewer analytical models have been developed for ductile materials. For small deformation elasto-plasticity and visco-plasticity, a majority of the analytical models are based on (a) variational estimates leading to Hashin-Strikman type bounds [6, 7, 8], (b) self consistent schemes [9] and (c) Mori-Tanaka methods [10, 11, 12] tend to oversimplify the morphological and material characteristics of its constituents. For example, variational estimates are obtained with rigid inclusions in [8] by assuming a nonlinear elastic behavior for the plastic constituents to produce upper and lower bounds. These estimates produce only a lower bound if the second phase is a void but are ineffective when both phases are deformable. Self consistent and Mori Tanaka methods are based on the concept of the equivalent inclusion method introduced by Eshelby [13], where the actual microscopic nonlinear response is derived from an average macroscopic counterpart. These methods provide reasonably good estimates for the overall macroscopic behavior when the heterogeneities occupy low volume fraction. However, the self-consistent and Mori-Tanaka methods produce widely discrepant results [14] at higher volume fractions, even in the elastic range. These models are also deficient in treating arbitrary distributions of shapes, sizes and location of the second phase, that are frequently encountered in real heterogeneous materials. Furthermore,
true depiction of microscopic stresses and strains in the constituent phases cannot be obtained from these models.

For a better representation of state variables in the microstructure (and consequently the overall response) various numerical schemes have been developed. Broadly classified as Unit Cell models, they have used semi-numerical bounding methods [15], local field approaches [16, 17] and finite element methods [18, 19, 20, 21] to solve the micromechanics problem. These methods assume that the material is constituted of periodic repetition of unit cells that are identified as representative volume elements (RVE) of the microstructure. Semi-numerical bounding techniques have used displacement based Galerkin and assumed stress hybrid finite element methods, to generate bounds on the actual overall response of unit cells. In local field approaches, the unit cells are decomposed into subcells containing exactly one constituent phase, and nonlinear response is predicted based on averaged state variables within subcells. Complete finite element methods resort to a detailed discretization of the unit cell or RVE to generate near exact representation of the microscopic morphology and thereby, compute local variables and the corresponding macroscopic response. Most of these models also assume local periodicity conditions implying uniform dispersion of simple shaped heterogeneities in the microstructure. This assumption essentially reduces the representative volume element to its basic structural element or (BSE), which is often a single inclusion with its neighboring matrix. These simplified unit cells bear little relationship to the actual stereographic features for many materials. Despite overcoming most of the limitations of analytical methods, the local periodicity assumptions in these methods grossly idealize actual microstructures for many
engineering materials. Micrographs of real heterogeneous materials often exhibit arbitrariness in shape, size and location of the second phase and prediction of macroscopic response based on analysis of a single BSE is inappropriate. To circumvent these deficiencies, Suresh and coworkers [22, 20], McHugh et. al. [23], among others have made novel progress in computationally modeling discontinuously reinforced materials with a random spatial dispersion. In general large inclusion aggregates require a very high resolution of finite element mesh in these unit cells, that leads to enormous computational efforts making the model large and inefficient.

Another important aspect involved in the design of heterogeneous materials is their enhanced ductility without undergoing substantial damage. However, the brittle constituents used to strengthen many composite systems tend to fracture with increased straining of the microstructure. Damage of the brittle constituents can in turn propagate into the more ductile phases resulting in catastrophic failure of the material. The degree of this influence depends on morphological characteristics like size, shape, orientation and spatial distribution of heterogeneities, and on constituent material properties. Drawbacks related to reliability and durability of heterogeneous materials have led to extreme caution in their applications to high performance structures. Rigorous fundamental studies, reflecting details of actual heterogeneous microstructures are therefore indispensable for understanding the effect of morphology on evolving state and material variables.
Within the framework of continuum damage mechanics, two distinct approaches, namely the phenomenological (see Kachanov[24] for a complete review) and micromechanical (see Talreja[25] and Nemat Nasser & Hori [26] for a complete review) approaches have evolved to analyze damage evolution in brittle single phase materials. Motivated by experimental observations, the phenomenological theories [27, 28, 29] introduce a set of scalar or tensor damage evolution parameters as internal variables in the constitutive requirements of irreversible thermodynamics processes (see [32, 33, 34] for details), with their growth determined by appropriate evolution laws. Consequently, the solid that is highly heterogeneous in the mesoscale is treated as a homogeneous continuum at the macroscale. Although these models have been popular for their relative simplicity in representing underlying physical complexities, the empirical treatment of morphological effects such as spatial distribution, size effects makes their application to many materials questionable [30, 31]. Proper choices of internal damage variables, like its tensorial representation and evolution characteristics are also non-trivial. On the other hand, micromechanical theories employ continuum mechanics principles at the microscopic level to predict overall constitutive response at the macroscopic level [35, 36, 38]. While some of these models [35] provide reasonable predictions of overall properties for a dilute distribution of damage entities, others [36, 38] attempt to analyze the interaction effects between damage entities introduced by the morphological characteristics of the microstructure. Recently, novel approaches to integrate micromechanical/computational approaches at the microscale with phenomenological approaches in the macroscale have also been proposed [30, 31, 40, 39]. While many of these methods can model damage in brittle (i.e. elastic) homogeneous (i.e. single phase) materials, far fewer analytical models
are available with the introduction of ductility and/or second phase geometries into the microstructure. Small scale yielding solutions using asymptotic analysis for a single bi-material interface due to Shih & Asaro [41] and Hutchinson et al. [42] are notable exceptions.

Alternatively, evolving damage in heterogeneous media with a mixture of ductile/brittle constituents have been modeled using unit cell methods. Notable among these are finite element implementations by Tvergaard[43], Bao[44], Hom[45], Suresh et al. [46] and Needleman et al. [47]. In [43, 44, 45, 46], simple microstructures with pre-damaged second phase heterogeneities are discretized into a conventional finite element mesh. In [47] a finite element mesh which allows for crack growth by element separation has been used to simulate the microscale unit cell. Finite element analysis of the unit cells are then used to explain underlying microstructural phenomenon that effect growth of plastic deformations near the crack tip [43, 46, 45, 47] as well as their implications towards overall weakening of the composite [43, 44, 47]. While these models provide valuable insights into the actual microstructural damage processes that cause failure in heterogeneous materials, the computational effort involved in modeling simple microstructures makes their implementation for random morphologies all but impossible. Further, due to the transient nature of damaging material morphologies, some of these models would require time wasting user interference in order to model progressive failure of the microstructures.

Experimental evidence of actual heterogeneous materials, however indicates that microstructural morphology can play a vital role in the structural failure of these materials. Scanning electron microscopy of damaged microstructures by Hunt et al. [48, 49], Kiser & Zok[50], Davidson [51] and Majumdar & coworkers [52] show particle
distribution, size and shape can significantly alter the extent of microstructural damage and the ensuing onset of material failure. Complete particle damage assumed in many computational models are usually a rarity in actual microstructure [49, 50, 51] and subsequent straining of the matrix material can be significantly influenced by the evolving local morphology of the damaged particles [51, 52]. Consequently, simplified microstructural representations of conventional unit cell models provide incomplete information into the phenomena that trigger the failure of actual heterogeneous materials. Further, experimental evidence [51, 52] also indicate that damage in the particles is usually evolving with the microscopic load on the constituents, making material modeling using conventional finite element schemes unattractive.

1.2 Scope of Proposed Research

In this thesis, a Voronoi Cell Finite Element Method (VCFEM) is innovated for the analysis of damage/undamaged random heterogeneous media. In this method, the finite element mesh evolves naturally by Dirichlet Tessellation of a representative microstructure. This is a process of subdivision of space, determined by a set of points, such that each point has associated with it a region that is closest to it than to any other. A mesh generator accounting for arbitrariness in shape, size and spatial distribution of inclusions has been developed by Ghosh and Mukhopadhyay [56]. Tessellation of a microstructural representative material element (RME) discretizes the domain into a network of multi-sided convex “Voronoi” polygons or cells. Each Voronoi cell contains one second phase inclusion at most, as shown in figure 2.1. Small deformation, elastic-plastic analysis of the 2-dimensional voronoi cell finite element
mesh is used to study the microscale/macroscale deformations of actual heterogeneous materials. Damage in the microstructure is introduced through cracking of particles triggered by a microscopic load levels in the heterogeneities. Consequently, the computational model will be capable of accounting for evolving damage in the real heterogeneous materials without user interference during the implementation phase of the finite element code. Numerical validation of VCFEM will be demonstrated through comparisons with analytical and traditional computational models. Effectiveness of VCFEM to model damage actual heterogeneous microstructures and its implications towards material failure will also be discussed.

While the primary focus of this thesis is geared towards the development of an efficient computational scheme for analyzing random microstructures, statistical correlation of damage evolution with geometric characteristics of the material morphology will also be examined in this thesis. Indeed, tessellation methods were introduced by Richmond and coworkers [53, 54, 22, 48] for quantitative characterization of micrographs obtained from automatic image analysis systems. Consequently, VCFEM provides a natural interface to link quantitative metallography with deformation analysis. Effect of particle shape, size and distribution on the failure of materials will be analyzed through computer simulated microstructures and there implication towards the design of actual materials examined.

1.3 Organization of the Thesis

The thesis has been divided into 7 chapters. In Chapter 2, variational formulation and various aspects of the computational scheme for undamaged heterogeneous media is presented. Numerical validation for undamaged media is presented in Chapter 3.
Extensions of the finite element scheme for damaged heterogeneous media are developed in Chapter 4. Numerical validation of VCFEM for damaged media is presented in Chapter 5. In Chapter 6, VCFE analysis of random microstructures and their link with quantitative metallography is studied. Capabilities of the developed computational model and possible improvements are discussed in the concluding chapter. Each chapter begins with a brief introduction to the essential features analyzed in that chapter. This is followed by main body consisting of theoretical developments and/or numerical results. A brief set of conclusions at the end of each chapter is used to introduce the reader to the next chapter.
CHAPTER 2

VORONOI CELL FINITE ELEMENT METHOD FOR UNDAMAGED RANDOM HETEROGENEOUS MEDIA

2.1 Introduction

In the Voronoi Cell Finite Element Method (VCFEM), the finite element mesh evolves naturally by Dirichlet Tessellation of a representative microstructure. Tessellation of a microstructural representative material element (RME) discretizes the domain into a network of multi-sided convex "Voronoi" polygons or cells. Each Voronoi cell contains one second phase inclusion at most, as shown in figure (2.1). Voronoi cells resulting from Dirichlet tessellation of a heterogeneous microstructure make rather unconventional elements, due to the arbitrariness in the number of sides. The application of conventional displacement-based finite element methods to these elements, suffer from difficulties associated with interelement displacement compatibility and rank deficiencies of the stiffness matrix. The Voronoi Cell finite element model developed by Ghosh and coworkers [55, 56, 57, 58, 59] avoids these difficulties by invoking the assumed stress hybrid method introduced by Pian [62]. In this formulation, independent assumptions are made on an equilibrated stress field in the interior of each element and a compatible displacement field on the element boundary. Small
deformation, elastic-plastic analysis of materials, embedded with second phase inclusions, has shown significant promise with this method [55, 56]. The developments, for rate independent $J_2$ flow theory, are based on the generalized Hu-Washizu principle originally proposed by Atluri [63, 64]. In this chapter, a detailed formulation of the Voronoi cell finite element method for undamaged heterogeneous media is presented. Variational principles for the VCFEM, element field representations, weak form of the assumed stress hybrid variational, and numerical aspects of the finite element scheme are discussed to provide the reader with a comprehensive introduction to the VCFEM. Many of the concepts presented here will be used in Chapter 4 as a basis for the development of VCFEM for damaged heterogeneous media.

2.2 Variational principle with assumed stress hybrid method

Consider a typical representative material element (RME), denoted as $\Omega$ in figure (2.1a), corresponding to the smallest portion of a microstructure that represents the local microscopic behavior at a point in a structure. The heterogeneous domain $\Omega$ is discretized by Dirichlet Tessellation procedure into $N$ Voronoi cells or VCFEs, based on the location, shape and size of the $N$ heterogeneities. The matrix phase in each Voronoi cell is denoted by $\Omega_m$ and the second phase (void or inclusion) is denoted by $\Omega_c$. Effectively, each Voronoi cell element may be identified as a basic structural element or BSE, which is defined as the smallest element of the microstructure reflecting its basic constituent characteristics (see figure 2.1b). Each element boundary $\partial \Omega_c$ is assumed to be comprised of a prescribed traction boundary $\Gamma_{tm}$, a prescribed displacement boundary $\Gamma_{um}$, and an interelement boundary $\Gamma_m$, i.e. $\partial \Omega_c = \Gamma_{tm} \cup \Gamma_{um} \cup \Gamma_m$. 
It is further assumed that these are mutually disjoint, i.e. $\Gamma_{tm} \cap \Gamma_{um} \cap \Gamma_m = \emptyset$. The matrix-second phase interface $\partial \Omega_e$ has an outward normal $n^e$, while $n^e$ is the outward normal to $\partial \Omega_e$. An incremental finite element formulation is invoked to account for the evolutionary constitutive equations in rate independent plasticity. At the beginning of an increment or step (say increment $p$), let $\sigma$ be an equilibrated stress field and $\varepsilon(\sigma, \text{loading path})$ the associated strain field in $\Omega_e$. Let $u$ and $u'$ denote respectively compatible displacement fields on the element boundary $\partial \Omega_e$ and the second phase boundary $\partial \Omega_c$. In the $p$-th step, $\Delta \sigma$ corresponds to an equilibrated stress increment in $\Omega_e$, $\Delta u$ and $\Delta u'$ correspond respectively to compatible displacement increments on the boundaries $\partial \Omega_e$ and $\partial \Omega_c$, and $\Delta t$ corresponds to the traction increment on $\Gamma_{tm}$. The resulting incremental problem is solved by using the two field assumed stress hybrid variational principle, derived from an element energy functional of the form:

$$
\Pi_e(\Delta \sigma, \Delta u) = - \int_{\Omega_e} \Delta B(\sigma, \Delta \sigma) \, d\Omega - \int_{\Omega_e} \varepsilon : \Delta \sigma \, d\Omega \\
+ \int_{\partial \Omega_e} (\sigma + \Delta \sigma) \cdot n^e \cdot (u + \Delta u) \, d\Omega - \int_{\Gamma_{tm}} (\bar{t} + \Delta \bar{t}) \cdot (u + \Delta u) \, d\Gamma \\
- \int_{\partial \Omega_c} (\sigma^m + \Delta \sigma^m - \sigma^c - \Delta \sigma^c) \cdot n^c \cdot (u' + \Delta u') \, d\Omega \quad (2.1)
$$

where $\Delta B$ is the increment in complimentary energy density of the element and the superscripts $m$ and $c$ represent respectively the matrix and second phase parts of the Voronoi cell element. The total energy functional for the entire domain is obtained by adding the element functionals as

$$
\Pi = \sum_{e=1}^{N} \Pi_e \quad (2.2)
$$
The first variation of $\Pi_\epsilon$ with respect to the stress increments $\Delta\sigma$ results in the kinematic condition as the Euler equation,

$$\nabla \Delta u = \Delta \epsilon \quad \text{in} \quad \Omega_\epsilon \quad (2.3)$$

while the first variation of $\Pi$ with respect to the independent boundary displacement increments $\Delta u$ and $\Delta u'$ yields traction conditions as Euler equations,

$$\begin{align*}
(\sigma + \Delta \sigma) \cdot n^{++} &= -(\sigma + \Delta \sigma) \cdot n^{--} \quad \text{on} \quad \Gamma_m \quad \text{Interelement traction reciprocity}\quad (2.4) \\
(\sigma + \Delta \sigma) \cdot n^e &= \dot{t} + \Delta t \quad \text{on} \quad \Gamma_{tm} \quad \text{Traction boundary conditions} (2.5) \\
(\sigma^e + \Delta \sigma^e) \cdot n^e &= (\sigma^m + \Delta \sigma^m) \cdot n^e \quad \text{on} \quad \partial \Omega_c \quad \text{Interface traction reciprocity}\quad (2.6)
\end{align*}$$

where, $+$ and $-$ denote neighboring element on $\Gamma_m$. The apriori assumptions on equilibrated stress increments $\Delta\sigma$ and constitutive relationships (through the complimentary energy density $\Delta B$), along with the Euler equations (2.3, 2.4, 2.5 and 2.6) completely define the initial value problem in the $p$-th increment.

### 2.3 Element formulations and assumptions

#### 2.3.1 Shape Based Stress Representations

The Voronoi cell finite element method (VCFEM) entails independent assumptions on (a) an equilibrated incremental stress field in the interior of the cell element $\Omega_e$ and on (b) a compatible incremental displacement fields on both element boundary $\partial\Omega$ and second phase boundary $\partial \Omega_c$. Furthermore, independent assumptions on stress increments $\Delta\sigma$ can be made in the matrix and heterogeneity phases so as to accommodate stress jumps across the interface. Use of Airy's stress functions $\Phi(x, y)$. 

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Figure 2.1: (a) Dirichlet Tessellation of a Representative Material Element into Voronoi Cells (b) Typical Voronoi Cell Representing the Basic Structural Element

in which $\Delta \sigma$ is expressed as,

$$
\Delta \sigma_{xx} = \frac{\partial^2 \Phi}{\partial y^2}, \quad \Delta \sigma_{yy} = \frac{\partial^2 \Phi}{\partial x^2}, \quad \Delta \sigma_{xy} = -\frac{\partial^2 \Phi}{\partial x \partial y}
$$

(2.7)

to derive equilibrated stress-increments is a convenient method in two-dimensional analysis. Different expressions may be assumed for $\Phi$ in the matrix and inclusion phases resulting in a discontinuous stress field across the interface of the Voronoi cell.

For example, a 4th order complete polynomial expansion of $\Phi^m$ may be assumed to give the stress increments in the matrix phase as

$$
\begin{bmatrix}
\Delta \sigma_{xx}^m \\
\Delta \sigma_{yy}^m \\
\Delta \sigma_{xy}^m
\end{bmatrix} =
\begin{bmatrix}
1 & y & 0 & 0 & 0 & x & 0 \\
0 & 0 & 1 & x & 0 & 0 & y \\
0 & 0 & 0 & 0 & 1 & y & -x
\end{bmatrix}
\begin{bmatrix}
\Delta \beta_1^m \\
\Delta \beta_2^m \\
\Delta \beta_3^m
\end{bmatrix}
$$

(2.8)

where $\{\Delta \beta^m\}$'s correspond to a set of stress coefficients that are determined as part of the finite element solutions. In general, the stress functions can be arbitrary functions.
of location, yielding stress increments in the form

\[
\{ \Delta \sigma^m \} = \left[ P^m(x, y) \right] \{ \Delta \beta^m \}
\]

\[
\{ \Delta \sigma^c \} = \left[ P^c(x, y) \right] \{ \Delta \beta^c \}
\]  

(2.9)

An important criterion, affecting the convergence Voronoi cell elements[55, 60], is the proper representation of stress fields in each of the constituent phases. A discussion of the essential features in the stress functions is presented next.

Problems of stress concentrations around voids have been traditionally handled by the use of specialized stress functions accounting for its shape. Analytical solutions by Muskhelishvili [65] and Sarin [66] use the Schwarz-Christoffel conformal mapping to transform an arbitrary shaped void into a circle in the complex plane. Analytic functions defined in the transformed plane are then used as the basis to generate accurate stress functions. Complex functions and conformal mapping techniques to construct trial stress functions in the assumed stress hybrid finite element method have been used by Tong et.al. [67] and Piltner [68] to solve elastic problems with cracks and holes. Their stress functions are chosen to satisfy apriori the biharmonic equation and hence provide a compatible strain field for linear elastic media only. However for non-linear constituent materials, a compatible strain field does not imply that the stress function satisfies the biharmonic equation (for example see Sarin[66]). Further, for elastic-plastic problems, incremental constitutive relationships are in general dependent on current stress levels. Current stress state in an element in turn depends on the the prescribed loading on the Voronoi cell boundary. Consequently, an explicit
form for the stress function that apriori satisfies compatibility conditions for any prescribed loading on the Voronoi cell boundary is all but impossible.

On the other hand, for the assumed stress hybrid functional used in section 2.2, strain-displacement or kinematic relationships are satisfied aposteriori as euler equation (2.3). It is therefore unnecessary for the stress functions to assume any form dictated by compatibility considerations. Matrix stress functions can now be derived from a more basic set of requirements dictated by the micromechanics of heterogeneous media, namely traction reciprocity conditions in equation (2.5). Three different conditions that are indispensable in this regard are:

1. Stress functions should, in some way, account for the shape of the heterogeneity.

2. Effects of the heterogeneity shape for the matrix stress functions should vanish at large distances from the interface.

3. The shape effects in matrix stress functions should facilitate traction reciprocity at the interface.

For both composite and porous materials, the first two considerations imply that the shape effect should be dominant near the interface, but vanish in the far-field. The third condition, for composite materials is intended to counteract interface tractions caused by the inclusion, while reduce it to zero interface tractions for porous materials.

Consider a a typical heterogeneity (void or inclusion) embedded in the matrix of a Voronoi cell as shown in figure (2.1b). Suppose that equation of the interface $\partial \Omega_c$ can be expressed in terms of polar coordinates as $g(r, \theta) = 0$, where the $r$ coordinate
is measured from the centroid of the heterogeneity. A Fourier series expansion for \( r \) in terms of the polar angle \( \theta \) may be expressed as:

\[
r = a_o + \sum_n a_n \cos(n\theta) + \sum_n b_n \sin(n\theta) \quad \text{on } \partial \Omega_c
\]  

where the Fourier coefficients \( a_n \) and \( b_n \) are given as:

\[
a_o = \frac{1}{2\pi} \int_{\partial \Omega_c} r \, d\Omega
\]

\[
a_n = \frac{1}{\pi} \int_{\partial \Omega_c} r \cos(n\theta) \, d\Omega \quad n = 1, 2, \cdots
\]

\[
b_n = \frac{1}{\pi} \int_{\partial \Omega_c} r \sin(n\theta) \, d\Omega \quad n = 1, 2, \cdots
\]

The interface equation may then be expressed from (2.10) as,

\[
g(r, \theta) = f - \frac{r}{a_0} - \sum_n \frac{a_n}{a_0} \cos(n\theta) - \sum_n \frac{b_n}{a_0} \sin(n\theta) = 0 \quad (2.11)
\]

Here \( f \) corresponds to a function that transforms any arbitrary shaped interface to an unit circle, since \( f(x, y) = 1 \) on \( \partial \Omega_c \). The mapped function \( f(r, \theta) \) may be thought of as a specialized radial coordinate with the property \( f \to 0 \) as \( (x, y) \to \infty \). This function is now used to construct reciprocal stress functions, that enrich a purely polynomial stress field, based on the shape of the shape of the interface. For each term \( x^p y^q \), in the polynomial stress function \( \Phi_{poly}^m = \sum_{p,q} \Delta \beta_{pq}^m x^p y^q \), a set of reciprocal counterparts \( x^p y^q(\frac{\Delta \beta_{pq1}^m}{f_{p+q}} + \frac{\Delta \beta_{pq2}^m}{f_{p+q+1}} + \cdots) \) result in a reciprocal stress function \( \Phi_{rec}^m \) of the form:

\[
\Phi_{rec}^m = \sum_{p,q} x^p y^q(\frac{\Delta \beta_{pq1}^m}{f_{p+q}} + \frac{\Delta \beta_{pq2}^m}{f_{p+q+1}} + \cdots)
\]

Consequently, the enriched stress function in the matrix phase is written as:

\[
\Phi^m = \Phi_{poly}^m + \Phi_{rec}^m \quad (2.12)
\]
The increment of traction vector at a point \( \Delta t^m \), may be related to the stress function \( \Phi^m \) using equation (2.7) as:

\[
\Delta t_x^m = \frac{\partial \Phi^m}{\partial y}, \quad \Delta t_y^m = -\frac{\partial \Phi^m}{\partial x}
\]

Substituting equation (2.12) in the traction increments gives

\[
\begin{align*}
\Delta t_x^m &= \sum_{p,q} qx^py^{n-1}(\Delta \beta_{pq}^m + \sum_{i=p+q}^{\infty} \Delta \beta_{pq,i}^m \frac{1}{f^i}) - \sum_{p,q} x^py^q \sum_{i=p+q}^{\infty} \Delta \beta_{pq,i}^m \frac{1}{f^i+1} \frac{\partial f}{\partial y} \\
\Delta t_y^m &= -\sum_{p,q} px^{m-1}y^q(\Delta \beta_{pq}^m + \sum_{i=p+q}^{\infty} \Delta \beta_{pq,i}^m \frac{1}{f^i}) + \sum_{p,q} x^py^q \sum_{i=p+q}^{\infty} \Delta \beta_{pq,i}^m \frac{1}{f^i+1} \frac{\partial f}{\partial x}
\end{align*}
\]

(2.13)

Coefficients of the reciprocal stress function \( \Delta \beta_{pq,i}^m \), in the first set of terms in equation (2.13), add flexibility to polynomial coefficients \( \Delta \beta_{pq}^m \) in the stress expansions by providing for matching tractions at the interface \( (f = 1) \). The gradient of \( f \) in second set of terms account for the shape of the interface. Terms produced by the reciprocal function in equation (2.13) have negligible effects on the traction vector far away from the heterogeneity, on account of \( f \) becoming extremely large. In other words, the far-field tractions are produced predominantly by polynomial terms in the stress function or the far field traction vectors are unaffected by shape of the heterogeneity. Stress increments in the matrix phase of the Voronoi cell are obtained from the traction increments by using equation (2.7) as:

\[
\begin{align*}
\begin{bmatrix}
\Delta \sigma_{xx}^m \\
\Delta \sigma_{yy}^m \\
\Delta \sigma_{xy}^m
\end{bmatrix}
&= \begin{bmatrix}
\sum_{p,q} \frac{\partial^2(z^p y^q)}{\partial y^2} \Delta \beta_{pq}^m + \sum_{p,q,i} \frac{\partial^2(z^p y^q f^i)}{\partial x^2} \Delta \beta_{pq,i}^m \\
\sum_{p,q} \frac{\partial^2(z^p y^q)}{\partial x^2} \Delta \beta_{pq}^m + \sum_{p,q,i} \frac{\partial^2(z^p y^q f^i)}{\partial x^2} \Delta \beta_{pq,i}^m \\
-\sum_{p,q} \frac{\partial^2(z^p y^q)}{\partial x \partial y} \Delta \beta_{pq}^m - \sum_{p,q,i} \frac{\partial^2(z^p y^q f^i)}{\partial x \partial y} \Delta \beta_{pq,i}^m
\end{bmatrix}
\end{align*}
\]

\[
= \begin{bmatrix}
\Delta \beta_{11}^m \\
\Delta \beta_{pq}^m \\
\Delta \beta_{pq}^m
\end{bmatrix}
+ \begin{bmatrix}
\Delta \beta_{11}^m \\
\Delta \beta_{pq}^m \\
\Delta \beta_{pq}^m
\end{bmatrix}
\]

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It should be noted that while stress functions used in equation (2.12) aid the satisfaction of traction reciprocity conditions along the inclusion/matrix interface, actual implementation of these conditions are effected aposteriori through euler equation (2.5) and hence as part of the finite element solution. Within a computational framework, the infinite asymptotic expansion of the reciprocal stress function $\Phi_{rec}^m$ is truncated to a finite number of terms, so that they are written as:

$$\Phi_{rec}^m = \sum_{p=1}^{P_m} \sum_{q=1}^{Q_m} \frac{1}{f_{p+q+i-1}}$$

A typical numerical transformation of a voided cell with a square shaped interface $\partial \Omega_e$ with a 20 term fourier expansion is shown in figure(2.2). The 20 term truncation of the infinite fourier expansion produces spikes at interface/element vertices in the
transformed domain. On the other hand, the inverse transformation of a unit circle from the transformed domain produces a smoothened square in the physical domain. Such an effect is more pronounced with the increased aspect ratios of the interface \( \partial \Omega_c \). Thus a larger number of terms need to be used in the fourier expansion, resulting in increased computational expense. Alternatively, explicit mapping functions derived from the Schwarz-Christoffel transformation [69, 65] also exhibit the properties \( f = 1 \) on \( \partial \Omega_c \) and \( \frac{1}{f} \rightarrow 0 \) as \( (x, y) \rightarrow \infty \). In this thesis, conformal mapping functions are used in the case of large aspect ratios (especially in the case of elliptical inclusions or cracks). As an example, for an elliptical interface of the form \( \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \) the Schwarz-Christoffel mapping function [65] can be written as \( f = \sqrt{|\psi^2 + \gamma^2|} \), where the transformed coordinates \( (\psi, \gamma) \) are obtained as solutions to the complex quadratic
equation,
\[(\psi + i\gamma)^2 - \frac{2(x + iy)(\psi + i\gamma)}{a + b} + \frac{a - b}{a + b} = 0\]

The resulting transformation of an elliptical interface \( \partial \Omega_c \) with \( \frac{a}{b} = 10 \) is shown in figure(2.3).

In the composite case, the stress functions \( \Phi^c \) within the heterogeneity are simply written in terms of polynomial functions as:

\[\Phi^c = \sum_{p,q} \Delta \beta^c x^p y^q \quad (2.16)\]

with stress increments \( \Delta \sigma^c \) derived as

\[
\begin{align*}
\begin{bmatrix}
\Delta \sigma^c_{xx} \\
\Delta \sigma^c_{yy} \\
\Delta \sigma^c_{xy}
\end{bmatrix}
&=
\begin{bmatrix}
\sum_{p,q} \frac{\partial^2 (x^p y^q)}{\partial x^2} \Delta \beta^c_{pq} \\
\sum_{p,q} \frac{\partial^2 (x^p y^q)}{\partial y^2} \Delta \beta^c_{pq} \\
- \sum_{p,q} \frac{\partial^2 (x^p y^q)}{\partial x \partial y} \Delta \beta^c_{pq}
\end{bmatrix}

&= [P^c] \{\Delta \beta^c\} 
\end{align*}
\]

**2.3.2 Displacement Field along Element Topologies**

Compatible displacement increments on the along element and interface boundaries are respectively generated by interpolation in terms of generalized values at the nodes on the element boundary \( \partial \Omega_e \) and interface boundary \( \partial \Omega_c \). Note that compatible displacement fields on the interface \( \partial \Omega_c \) imply perfect bonding in the case of composite materials. As an example, a linear interpolation of displacement increments on the boundary segment between the \( i \)th and \((i + 1)\)th nodal points may be expressed as,

\[
\{\Delta u\} = \begin{bmatrix}
\Delta u_x \\
\Delta u_y
\end{bmatrix}
= \begin{bmatrix}
1 - a/l_i & 0 & a/l_i & 0 \\
0 & 1 - a/l_i & 0 & a/l_i
\end{bmatrix}
\begin{bmatrix}
\Delta q_{2i-1} \\
\Delta q_{2i} \\
\Delta q_{2i+1} \\
\Delta q_{2i+2}
\end{bmatrix} 
\]

(2.18)
where \( l_i \) is the length of the line segment and \( a \) is the distance from the \( i \)-th node. Thus the displacement increments on the Voronoi cell boundary and the interface may be respectively written as,

\[
\{ \Delta u \} = [L'] \{ \Delta q \}
\]

\[
\{ \Delta u' \} = [L'] \{ \Delta q' \}
\]

(2.19)

where \( \{ \Delta q \} \) and \( \{ \Delta q' \} \) are generalized displacement increment vectors.

### 2.3.3 Weak Form of the Assumed Stress Hybrid Variational

Substituting element approximations for stresses (2.9), and displacements (2.19), in the energy functional (2.1), and setting the first variations with respect to the stress parameters \( \Delta \beta^m \) and \( \Delta \beta^c \) respectively to zero, results in the following two weak forms of the kinematic relations (2.3),

\[
\int_{\Omega_m} [P^m]^T \{ \epsilon + \Delta \epsilon \} d\Omega = \int_{\partial \Omega_m} [P^m]^T [n^e] [L^e] d\Omega \{ \Delta q \} - \int_{\partial \Omega_c} [P^m]^T [n^c] [L^c] d\Omega \{ \Delta q' \}
\]

\[
\int_{\Omega_c} [P^c]^T \{ \epsilon + \Delta \epsilon \} d\Omega = \int_{\partial \Omega_c} [P^c]^T [n^e] [L^e] d\Omega \{ \Delta q' \}
\]

(2.20)

For two-dimensional problems \([n^e] \) and \([n^c] \) are \((3 \times 2)\) matrices, consisting of the components of unit outward normals to the element boundary and interface respectively.

Thus

\[
[n(x)] = \begin{bmatrix}
 n_x(x) & 0 \\
 0 & n_y(x) \\
 n_y(x) & n_x(x)
\end{bmatrix}
\]

Furthermore, setting the first variation of the total energy functional in equation (2.2) with respect to increments in nodal displacements \( \Delta q \) and \( \Delta q' \), result in the weak form of the traction reciprocity conditions

\[
\sum_{\varepsilon=1}^{N} \left[ \int_{\partial \Omega_\varepsilon} [L^\varepsilon]^T [n^c]^T [P^m] d\Omega - \int_{\partial \Omega_\varepsilon} [L^\varepsilon]^T [n^e]^T [P^m] d\Omega \right] \left\{ \beta^m + \Delta \beta^m \right\} = \sum_{\varepsilon=1}^{N} \left[ \int_{\partial \Omega_\varepsilon} [L^\varepsilon]^T [n^e]^T [P^c] d\Omega \right] \left\{ \beta^c + \Delta \beta^c \right\}
\]
For an elastic-plastic material, the strain increments $\Delta \epsilon$ in equation (2.20) are non-linear functions of the current stress state $\sigma$ as well as of stress increments $\Delta \sigma$. Thus, the non-linear finite element equations (2.20) and (2.21) at the $p$-th increments have to be solved iteratively for the stress parameters $(\Delta \beta^m, \Delta \beta^p)$ and the nodal displacement increments $(\Delta q, \Delta q')$.

### 2.4 Constitutive Relations

In this thesis, the heterogeneity phase is assumed to be linear elastic. Constitutive dependence of the strain increments $\Delta \epsilon$ on the stress increments $\Delta \sigma$ can therefore be obtained from Hooke’s law as,

$$\Delta \epsilon = \frac{1 + \nu}{E} \Delta \sigma - \frac{\nu}{E} \Delta \delta$$

(2.22)

where, $E$ is the Young's modulus, $\nu$ is the Poisson’s ratio, $\Delta \sigma$ is the hydrostatic component of the stress increment $\Delta \sigma$ and $\delta$ is the Kronecker delta. The matrix phase of the RME is modeled through a rate independent small deformation elastoplastic constitutive relation, following $J_2$ flow theory with isotropic hardening [70, 71]. Constitutive relationships for such materials and aspects of the numerical integration are presented in this section.

#### 2.4.1 Constitutive equations for matrix material

For a material law obeying $J$-2 flow theory with isotropic hardening, an additive decomposition of the strain increments $\Delta \epsilon$ into an elastic part $\Delta \epsilon^e$ and a plastic part
\( \Delta e^p \) is assumed, giving

\[
\Delta e = \Delta e^e + \Delta e^p \tag{2.23}
\]

The elastic part of the strain increment tensor \( \Delta e^e \) is obtained through the linear elastic relationship outlined in equation (2.22). The plastic strain increments on the other hand are obtained through the integration of the associated flow rule. Consider the yield surface for a \( J_2 \) material in stress-space expressed as \( F = 0 \), with \( F \) written as:

\[
F = \sigma_m - H(e^p) = \sqrt{\frac{3}{2} \sigma' : \sigma'} - H(e^p) \tag{2.24}
\]

where \( \sigma' \) is the deviatoric stress tensor, \( \sigma_m \) is the radius of the flow surface or the effective stress, \( e^p = \sqrt{\frac{3}{2} e^p} : e^p \) is the effective plastic strain and \( H(e^p) \) is the isotropic hardening function. The plastic strain rate \( \dot{e}^p \) from the associated flow rule \( \dot{e}^p \approx \frac{\partial F}{\partial \sigma} \) can now be expressed as:

\[
\dot{e}^p = \dot{\lambda} \sigma'
\tag{2.25}
\]

where the non-negative flow parameter \( \dot{\lambda} \) is obtained from the Kuhn-Tucker conditions as:

\[
\dot{\lambda} \dot{F} = 0
\]

Since the plastic strain rate \( \dot{e}^p \) is dependent on the flow parameter \( \dot{\lambda} \) through the flow equation (2.25), the isotropic hardening function \( H(e^p) \) depends implicitly on the flow parameter \( \dot{\lambda} \). Consequently, for non-negative \( \dot{\lambda} \), the Kuhn-Tucker condition can be recast in the form:

\[
\dot{\lambda} = 0 \text{ if } \dot{\sigma}_m < 0 \quad \text{Elastic unloading}
\]

\[
\sigma_m + \int \dot{\sigma}_m = H(e^p + \int \dot{e}^p(\dot{\lambda})) \text{ if } \dot{\sigma}_m > 0 \quad \text{Neutral and plastic loading (2.26)}
\]
where the integrals are implemented over the current load step $p$. Numerical aspects of the integration scheme are considered next.

### 2.4.2 Numerical integration of constitutive relations

Numerical integration of the associated flow rule in equation (2.25) at the $p$th step through a generalized one-step Euler method can be written as:

$$
\Delta e^{pl}|_p = \Delta \lambda (\sigma'|_p + \alpha \Delta \sigma'|_p)
$$

where $\alpha \in [0,1]$. Ortiz and Popov [72] have shown the integration algorithm is stable for $\alpha \geq \frac{1}{2}$. Numerical evidence due to Simo et al. [73, 74] suggests that the backward euler algorithm with $\alpha = 1$ is most accurate and is implemented in this thesis. Substitution of the associated flow rule (2.27) with midstep parameter $\alpha = 1$ and the relationship $\Delta e^{pl} = \Delta \lambda (\sigma'|_p + \alpha \Delta \sigma'|_p)$ into the Kuhn-Tucker condition (2.26) results in the numerical equations:

$$
\Delta \lambda = 0 \text{ if } \Delta \sigma^p_m < 0 \quad \text{Elastic unloading}
$$

$$
\sigma_m + \Delta \sigma^p_m = H \left( \frac{3}{2} \Delta \lambda (\sigma^p_m + \Delta \sigma^p_m) \right) \text{ if } \Delta \sigma_m > 0 \quad \text{Neutral and plastic loading}
$$

For given stress increments $\Delta \sigma$ and arbitrary hardening functions $H(e^{pl})$ a regula falsi scheme is used to solve the implicit equation (2.28) to determine the flow parameter $\Delta \lambda$. The algorithm is summarized into the following steps:

- Assign $\Delta \lambda = 0$ and compute $\Delta \sigma^p_m$.
- If $\Delta \sigma^p_m \geq 0$ then {Neutral and plastic loading}
- Assign $\Delta \lambda_1 = 0$ and $F_1 = \Delta \sigma_m$. Set $i = 2$ and $\Delta \lambda = TOL$.

- Do while $|F_{i-1}| > \sigma_0 TOL \{ \text{Checking if yield surface equation } F = 0 \text{ is satisfied} \}
  
  * Calculate $\Delta \varepsilon_i^{pl} = \frac{\gamma}{2} \Delta \lambda (\sigma_m^p + \Delta \sigma_m^p)$. Also calculate $F_i = \Delta \sigma_m^p - H(\varepsilon_i^{pl}|_p + \Delta \varepsilon_i^{pl})$. \{Determining the yield surface $F_i$ at step $i$\}

  * Calculate $\Delta \lambda_{i+1} = \Delta \lambda_i - \frac{F_i}{F_i - F_{i-1}} (\Delta \lambda_i - \Delta \lambda_{i-1})$. \{The flow parameter $\Delta \lambda_{i+1}$ at step $i+1$ obtained as a linear correction to the flow parameter $\Delta \lambda_i$ at step $i$\}

  * Set $i = i + 1$  

- Enddo

- Set $\Delta \lambda = \Delta \lambda_i$

- Endif

- Determine $\Delta \varepsilon^e$ from Hooke’s law (2.22) and $\Delta \varepsilon^{pl}$ from the associated flow rule (2.27).

- Calculate $\Delta \varepsilon$ from the additive decomposition condition (2.23).

Numerical implementation requires computation of tangent operators through linearized forms of the constitutive relations. If $d\varepsilon$ is the first order correction to the current strain increment $\Delta \varepsilon$, and $d\sigma$ is the corresponding correction to the stress increment $\Delta \sigma$, the fourth order elastic-plastic compliance tensor (or tangent operator) $S$ is given by the relation

$$d\varepsilon = S : d\sigma$$
The elastic part of this equation is expressed as

\[ \text{de}^e = S_e : d\sigma \]

where the elastic compliance in obtained directly from equation (2.22) as:

\[ S_e = \frac{1 + \nu}{E} I - \frac{\nu}{E} \delta \otimes \delta \]

(2.29)

\( I \) in this equation is the fourth order identity tensor. The plastic part of the strain correction \( \text{de}^{pl} \) however requires a first order approximation \( d\lambda \) to the current flow parameter \( \Delta \lambda \), which for \( J_2 \) flow theory (see Hill [70]), takes the form

\[ \text{de}^{pl} = \frac{9}{4H} \frac{(\sigma + \Delta \sigma)' \otimes (\sigma + \Delta \sigma)'}{(\sigma_{eff}^p + \Delta \sigma_{eff}^p)^2} : d\sigma = S_{pl} : d\sigma \]

(2.30)

where \( H \) is a linearized hardening modulus. The elasto-plastic tangent operator \( S \) is obtained by adding equations (2.29) and (2.30) as

\[ S = S_e + S_{pl} \]

(2.31)

A linearized form of the incremental complementary energy functional \( \Delta B \) in equation (2.1) can now be expressed in terms of the tangent operator as

\[ dB(\sigma, d\sigma) = \frac{1}{2} d\sigma : S : d\sigma \]

(2.32)

Note that the elastic-plastic tangent operator \( S \) in equation (2.31) is positive definite since its components are individually positive definite. Both plane stress and plane strain conditions have been solved in an iterative manner by this basic algorithm.

2.5 Solution Method for the Weak Form

For rate independent plasticity, the strain increments \( \Delta e(\Delta \sigma, \sigma) \) in the \( p \)-th increment are nonlinear functions of the stress parameters \( \Delta \beta^m \) and \( \Delta \beta^c \) in the matrix
and the heterogeneity respectively. An iterative solution process is therefore invoked to solve equation (2.20) and evaluate the stress increments for given nodal displacement increments \( \{ \Delta q \} \) and \( \{ \Delta q' \} \). Let \( \{d\beta\}^i \) correspond to the correction to the value of \( \Delta \beta \) in the \( i \)-th iteration, i.e.

\[
\{ \Delta \beta^m \} = \{ \Delta \beta^m \}^i + \{ d\beta^m \}^i \\
\{ \Delta \beta^c \} = \{ \Delta \beta^c \}^i + \{ d\beta^c \}^i
\]

The kinematic equation (2.20) may then be linearized with respect to \( \Delta \beta \) to yield:

\[
\begin{bmatrix}
H_m & 0 \\
0 & H_c
\end{bmatrix}
\begin{bmatrix}
d\beta^m \\
d\beta^c
\end{bmatrix}^i = 
\begin{bmatrix}
G_e & -G_{cm} \\
0 & G_{cc}
\end{bmatrix}
\begin{bmatrix}
q + \Delta q \\
q' + \Delta q'
\end{bmatrix} - 
\begin{bmatrix}
\int_{\Omega_m}[P^m]^i\{\epsilon + \Delta \epsilon\}^i d\Omega \\
\int_{\Omega_c}[P^c]^i\{\epsilon + \Delta \epsilon\}^i d\Omega
\end{bmatrix}
\]

In a condensed form this can be restated as:

\[
[H] \{d\beta\}^i = [G] \{\Delta u\} - \begin{bmatrix}
\int_{\Omega_m}[P^m]^i\{\epsilon + \Delta \epsilon\}^i d\Omega \\
\int_{\Omega_c}[P^c]^i\{\epsilon + \Delta \epsilon\}^i d\Omega
\end{bmatrix} \forall \epsilon = 1 \cdots N \quad (2.34)
\]

where,

\[
[H_m] = \int_{\Omega_m}[P^m]^T[S][P^m]d\Omega , \quad [H_c] = \int_{\Omega_c}[P^c]^T[S][P^c]d\Omega \\
[G_e] = \int_{\partial \Omega_e}[P^m]^T[n^e][L^e]d\Omega , \quad [G_{cm}] = \int_{\partial \Omega_e}[P^m]^T[n^e][L^e]d\Omega \quad [G_{cc}] = \int_{\partial \Omega_e}[P^c]^T[n^e][L^e]d\Omega 
\]

and \([S(x, y)]\) is the instantaneous elastic-plastic tangent compliance tensor as derived in equation (2.31). The linearized matrix equation (2.34) is solved for the stress tensor parameters using a Quasi-Newton iterative solution procedure outlined in [75].

The above procedure of solving for the stresses take place within an iterative loop, in which the traction reciprocity conditions (2.21) are solved for the nodal displacement increments \( \{ \Delta q \} \) and \( \{ \Delta q' \} \). Proceeding in the same way as for stresses, let
\{dq\}^j correspond to the correction in \{Δq\} in the \(j\)-th iteration of (2.21), i.e.

\[
Δq = Δq^j + dq^j
\]

\[
Δq'^j = Δq'^j + dq'^j
\]

Substituting equation (2.34) in the weak form of the global traction reciprocity equation (2.21) and linearizing with respect to the displacement increment \{Δq\}, yields the following matrix equation:

\[
\sum_{e=1}^{N}[G]^T[H]^{-1}[G]\begin{bmatrix} dq \\ dq' \end{bmatrix}^j = \sum_{e=1}^{N}\left\{ \int_{\Gamma_{im}}[L]^T\{\xi + Δt\}dΩ \right\} - \sum_{e=1}^{N}\left[ \begin{bmatrix} \int_{\Gamma_e}[L_e]^T[n_e]^T[P_m]dΩ & 0 \\ -\int_{\Gamma_e}[L_e]^T[n_e]^T[P_m]dΩ & \int_{\Gamma_{ce}}[L_c]^T[n_c]^T[P_c]dΩ \end{bmatrix}\begin{bmatrix} β^m + Δβ^m \\ β^c + Δβ^c \end{bmatrix} \right]^j
\]

or in standard finite element notation

\[
\sum_{e=1}^{N}[K_e]\{du\}^j = \sum_{e=1}^{N}\{f_e\} - \sum_{e=1}^{N}\left[ \begin{bmatrix} \int_{\Gamma_e}[L_e]^T[n_e]^T[P_m]dΩ & 0 \\ -\int_{\Gamma_e}[L_e]^T[n_e]^T[P_m]dΩ & \int_{\Gamma_{ce}}[L_c]^T[n_c]^T[P_c]dΩ \end{bmatrix}\begin{bmatrix} β^m + Δβ^m \\ β^c + Δβ^c \end{bmatrix} \right]^j
\]

With known traction increments on \(Γ_{im}\) and displacement increments on \(Γ_{um}\), the linearized global traction reciprocity condition equation (2.36) is solved iteratively using the Quasi-Newton method [75] for the nodal displacement increments.

### 2.6 Numerical Aspects of VCFEM

In order to effectively implement the VCFEM in a computational environment, special care needs to be exercised on the numerical stability of the various matrix systems developed in the previous sections. Proper conditioning of matrices \([H_m]\) and \([H_c]\) to ensure their invertability, accurate numerical integration of \([H]\) matrices over
their respective domains, judicious choice on the number of stress parameters $\Delta \beta^m$ and $\Delta \beta^c$ to avoid rank insufficiencies in the stiffness matrix $[K_e]$ and suppression of rigid body modes in the deformation field of the interface can contribute considerably towards enhancing the accuracy of the resulting VCFEM solutions. Some of the essential features incorporated in the programming phase of VCFE code are presented next.

2.6.1 Scaled representation of stress function $\Phi$

Matrices $[H_m]$ and $[H_c]$ need to be inverted in order to evaluate the element stiffness matrix $[K_e]$. However, stress representations by polynomial expressions of cartesian coordinates with varied exponents are carried over to the $[H]$ matrices. Such terms can make disparate contributions to the $[H]$ matrices in their domains of integration. For example, a 6th order complete polynomial would result in both $O(x^6)$ and $O(1)$ terms in the $[H]$ matrix. For Voronoi cells far removed from the origin, contribution of $O(x^6)$ term is much larger than that of $O(1)$ term. Large differences among the various elements of the $[H]$ matrices can in turn lead to bad conditioning or poor invertability of these matrices. This can lead to considerable numerical inaccuracy in the resulting stiffness matrix. To circumvent this problem, Ghosh et.al. [55, 56] have used scaled polynomial stress functions in terms local element coordinates $(\xi, \eta)$. The linear mapping from the $(x, y)$ coordinate system is expressed as:

$$\xi = (x - x_c)/l$$

$$\eta = (y - y_c)/l$$
where \((x_c, y_c)\) are the centroidal coordinates of a Voronoi cell element and \(l\) is a scaling parameter given as:

\[
l = \sqrt{\max(x - x_c) \max(y - y_c)} \quad \forall (x, y) \in \partial \Omega_e
\]

The scaling to \((\xi, \eta)\), leads to an approximate range of variation \(-1 \leq \xi \leq 1\) and \(-1 \leq \eta \leq 1\) in most Voronoi cell elements. Note that this range is exactly true for square elements. As an example, a fourth order complete polynomial Airy’s function in terms of \((\xi, \eta)\) gives rise to:

\[
[P] = \begin{bmatrix}
1 & \eta & 0 & 0 & 0 & \xi & 0 \\
0 & 0 & 1 & \xi & 0 & 0 & \eta \\
0 & 0 & 0 & 0 & 1 & -\eta & -\xi
\end{bmatrix}
\]

or for a more general case,

\[
\Phi_{poly} = \sum_{p+q=1}^{m} \xi^p \eta^q \Delta \beta_{pq}
\]

Individual terms in the reciprocal stress functions \(\Phi_{rec}^m\) used in equation(2.15) are of the form \(\frac{\pi^{p,q}}{f^{p+q+i-1}}\). While the reciprocal terms \(\frac{1}{f^{p+q+i-1}}\) in the stress functions varies from \(1 \rightarrow 0\) and hence can be obtained to the desired numerical accuracy, the polynomial terms in the numerator can adversely affect the conditioning of the \([H_m]\) matrix. To avoid this problem, the polynomial terms in reciprocal stress function are also written in terms of the scaled coordinates \((\xi, \eta)\), so that,

\[
\Phi_{rec}^m = \sum_{p+q=1}^{M} \xi^p \eta^q \sum_{i=1}^{n} \frac{1}{f^{p+q+i-1}} \Delta \beta_{pq}^m
\]
Figure 2.4: Division algorithm for a typical voronoi Cell (a) Neighbor identification for cell nodes (b) Discretization of matrix and inclusion domains into quadrilaterals and triangles (c) Subdivision of quadrilaterals in the matrix for integration of reciprocal functions

Figure 2.5: Subdivision for a typical undamaged voronoi cell. Shaded elements are used in the inclusion domain
2.6.2 Numerical integration of element matrices in the two phases of the voronoi cell

Another factor that contributes to the convergence of the method is accurate domain integration to evaluate $[H_m]$ and $[H_c]$. For polynomial stress functions, these matrices are also polynomial functions of scaled coordinates $(\xi, \eta)$. Numerical integration of these functions are performed by dividing the matrix domain $\Omega_m$ and the inclusion domain $\Omega_c$ into quadrilaterals and triangles. For undamaged heterogeneities, the inclusion domain $\Omega_c$ is a simply connected convex area whose division is easily accomplished. The matrix domain $\Omega_m$, however, is multiply connected and a general algorithm for subdividing it into quadrilaterals is shown in figure (2.4). The essential steps involved in the division are:

- Identify nodes on the interface $\partial\Omega_c$ that are closest to nodes on the voronoi cell boundary $\partial\Omega_c$. In figure (2.4a) nodes on the cell boundary are identified with arabic numerals, and their closest neighbors on the interface boundary by roman numerals.

- Join nodes on cell boundary with their closest neighbors. In figure (2.4b) this process is denoted by a solid line. Also join any unconnected nodes on the inclusion boundary (marked by a “x” in figure 2.4a) to the cell boundary. In figure (2.4b) this process is denoted by a dotted line.

- Finally, undamaged inclusions are subdivided into triangles by joining the inclusion nodes onto the inclusion center as shown in figure (2.4b).

Integration is now to be performed by using appropriate gaussian quadrature rule on the divided quadrilaterals/triangles, with the number of gauss points determined.
from the functional representation of individual terms in $[H]$. Using equations (2.38 and 2.17) in equation (2.35), the highest polynomial order for matrix $[H_e]$ is easily shown to be $O(2(m - 2))$. For the triangles dividing the inclusion domain $\Omega_e$, the appropriate number gauss points as per [76] is chosen to be $n_{gauss} = m - 1$. On the other hand, the $[H_m]$ matrix comprises of both polynomial and reciprocal terms. Of these, the sharpest gradients are exhibited by the reciprocal terms. Substituting of equations (2.39 and 2.14) in equation(2.35) the maximum reciprocal order in $[H_m]$ is seen to be $O(\frac{1}{\ell (m+n+1)})$. From figure (2.4b), for divided quadrilaterals in the matrix domain $\Omega_m$, most of the variation in the reciprocal mapping function $f$ occurs along lines joining voronoi cell nodes with inclusion nodes. Typically, for stiffer inclusions $m = 2..4$ and $n = 3$. Thus, for $M = 2$ and $n = 3$, most of the the variation in $\frac{1}{\ell (m+n+1)}$ will occurs near the inclusion interface ($f \approx 1..1.1$) with negligible effect as the Voronoi cell boundary is approached. It is therefore assumed that subdivision of these lines, with a larger number of integration points concentrated near the interface, is sufficient to accurately integrate functions of the order $O(\frac{1}{\ell (m+n+1)})$ along these lines. The adaptive scheme employed in subdividing individual quadrilaterals in the matrix domain $\Omega_e$ is shown in figure (2.4c). The procedure can be summarized as:

- Identify 5 points on the line joining the inclusion nodes with voronoi cell boundary (starting with the inclusion node) such that $f_{i+1}^{2(m+n+1)} \geq f_i^{2(m+n+1)}$. These are denoted by a "x" and a number in figure (2.4c).

- Join the points "x" with the same number to subdivide the original quadrilateral into 4 smaller quadrilateral. The resulting smaller quadrilaterals are marked with roman numerals in figure (2.4c).
• Along the radial direction viz. along the lines joining the inclusion nodes with the voronoi cell boundary, \( n_{\text{gauss}}^r = 5 \) for quadrilateral I and \( n_{\text{gauss}}^r = 3 \) for quadrilateral II, III, and IV.

• Along the polar direction viz. along lines joining points "x" of the same number \( n_{\text{gauss}}^\theta = 4 \) for all quadrilaterals.

The scheme results in 56 integration points \( \Sigma n_{\text{gauss}}^\theta n_{\text{gauss}}^r \) for the set of 4 quadrilaterals marked I, II, III, and IV in figure (2.4c). The final set of quadrilaterals used in the integration scheme of a typical voronoi cell is shown in figure (2.5).

2.6.3 Minimum stress coefficients for rank sufficiency of \([K]_e\)

An essential feature adversely affecting the accuracy of many finite element methods [77, 78] is the presence of spurious zero energy modes or hourglass modes in the element stiffness. The internal energy of all element stiffness matrices vanishes for rigid-body deformations on its boundary. However, certain spurious deformation (non-rigid body) modes may also contribute zero energy to the element and the resulting stiffness matrix suffers becomes rank insufficient. For a VCFE, the internal energy \( IE \) of the linearized stiffness matrix in equation (2.36) can be simplified using equation (2.33) to the form,

\[
IE = \frac{1}{2} \{d\beta^m\}^T [H_m] \{d\beta^m\} + \{d\beta^c\}^T [H_c] \{d\beta^c\}
\]

with

\[
\{d\beta\} = [H_m]^{-1} ([G_e]\{dq\} - [G_{cm}]\{dq'\})
\]

35
and

\[\{d\beta_c\} = [H_c]^{-1}[G_{cc}]{dq'}\]

For positive definite \([H_m]\) and \([H_c]\), the internal energy is zero only if each of the stress coefficients are individually zero. Setting \(\{d\beta_c\}\) to zero it can be seen that the inclusion contribution is zero only if,

\[\{G_{cc}\}{dq'} = 0\]

If the number of nodes on the inclusion were denoted by \(s'\) (corresponding to the number of columns in \([G]\)cc) and the number of stress coefficients in the inclusion were denoted by \(r'\) (corresponding to the number of rows in \([G]\)cc), than the necessary condition for \([G_{cc}]{dq'} = 0\) for no more than the 3 in-plane rigid body modes can be written as:

\[r' \geq 2s' - 3 \quad (2.40)\]

Further, if \({dq'}\) is a rigid body displacement, then the resulting internal energy \(IE_1 = \frac{1}{2}\{d\beta^m\}^T[H_m]\{d\beta^m\}\) for a heterogeneous element goes to zero if

\[\{G\}e{dq} = 0\]

If the number of nodes on the Voronoi cell were denoted by \(s\) (corresponding to the number of columns in \([G]\)e) and the number of stress coefficients in the inclusion were denoted by \(r\) (corresponding to the number of rows in \([G]\)e), than the necessary condition for \([G_e]{dq} = 0\) for no more than the 3 in-plane rigid body modes can be written as:

\[r \geq 2s - 3 \quad (2.41)\]

These two conditions (2.40 and 2.41) provide the necessary number of stress coefficients in terms of the the number of nodes on the inclusion and cell boundaries in
order to suppress hourglass modes in the element stiffness. Sufficiency condition is ensured by numerically ascertaining the invertability of the \([H_m]\) and \([H_c]\) matrices in the computational phase of VCFEM implementation.

2.6.4 Constraining rigid-body modes in the inclusion interface

In most finite element schemes, rigid-body modes of deformation are specified by applying suitable constraints on the boundary of the domain. Since the finite element mesh forms an interconnected network, the specified rigid-body nodes are automatically transferred to all of the networked nodes in the finite element mesh. However in the VCFEM, the interface nodes are in general not topologically connected to the element nodes. It is therefore necessary to specify the rigid-body modes for the displacement field \(\{q'\}\) on the interface. This implies that for \([K_e]\) to be invertible, 3 additional constraints should be imposed. These constraints are derived by equating rigid body modes on the interface to the rigid body modes on the element boundary. For a \(s\) sided Voronoi cell with coordinates \((x_i, y_i)\), any rigid-body mode of deformation can be expressed as:

\[
\{dq^R\}_e = \begin{bmatrix}
1 & 0 & -y_1 \\
0 & 1 & x_1 \\
1 & 0 & -y_2 \\
0 & 1 & x_2 \\
\vdots & \vdots & \vdots \\
1 & 0 & -y_s \\
0 & 1 & x_s \\
\end{bmatrix} \begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\end{bmatrix} = [\phi] \{\alpha\}
\]  

(2.42)
In order to calculate the interface rigid-body modes, consider the interface displacement field \( \{ dq' \} \) to be the sum of a rigid body mode and a purely deformation mode.

\[
\{ dq' \} = [\phi'][\alpha] + \{ dq' \}_\text{def} \tag{2.43}
\]

where \( \{ dq' \}_\text{def} \) is the pure deformation part of \( \{ dq' \} \). Since the pure deformation mode is orthogonal to the space spanned by rigid body modes, \( \{ dq' \}_\text{def} \) lies in the null space of \( [\phi]' \), i.e.

\[
[\phi]'^T \{ dq' \}_\text{def} = \{ 0 \}
\]

Here \( [\phi]' \) corresponds to the \( [\phi] \) matrix in equation (2.42) with components in terms of interface coordinates \( (x'_i, y'_i) \) and \( i = 1..s' \). Written explicitly, this corresponds to the following set of algebraic equations.

\[
\begin{align*}
\sum_{i=1}^{s'} u_{i,\text{def}} &= 0 \\
\sum_{i=1}^{s'} v_{i,\text{def}} &= 0 \\
(-u_1' y_1' + v_1' x_1') + (-u_2' y_2' + v_2' x_2') + \cdots + (-u_n' y_n' + v_n' x_n') &= 0
\end{align*}
\]

The first two constraints imply that there is at least one point on \( \partial \Omega_c \) for which the \( x \)- and \( y \)-components of pure deformation field are zero. The third constraint postulates that in a pure deformation mode field, at least one point on \( \partial \Omega_c \) has a zero rotation with respect to the origin. The equation for expressing the equivalence of rigid body modes on the interface \( \partial \Omega_c \) and element boundary \( \partial \Omega_e \) is then obtained from equation (2.43) as:

\[
\{ [\phi]'^T [\phi]' \}^{-1} \{ dq' \} = \{ [\phi]'^T [\phi] \}^{-1} \{ dq \}
\]

or

\[
[\Phi] \begin{bmatrix} dq' \\ dq \end{bmatrix} = \{ 0 \} \tag{2.44}
\]

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This constraint needs to be imposed for making the element stiffness $[K_e]$ nonsingular. This is achieved by adding the constraint (2.44) as lagrange multipliers to the element internal energy $IE$: 

$$IE_{RME} = \sum_{e=1}^{N}(IE + \{\lambda\}^T[\Phi]\left\{\begin{array}{c} dq \\ dq' \end{array}\right\})$$

Addition of the constraint modifies the original stiffness matrix to the form

$$\begin{bmatrix} 0 & \Phi \\ \Phi^T & K_e \end{bmatrix}\left\{\begin{array}{c} \lambda \\ u \end{array}\right\} = \left\{\begin{array}{c} 0 \\ f_e^* \end{array}\right\}$$

which is solved using a perturbed lagrangian method suggested by Simo et.al.[79].

### 2.7 Conclusions

A theoretical framework for the development of VCFEM for undamaged heterogeneous media has been presented in this chapter. Assumed stress hybrid variational principle used by VCFEM, element approximations, constitutive relationships for non-linear materials, solution methodology for the resulting weak form and numerical aspects of VCFEM implementation are discussed. VCFEM for undamaged media is validated by computational experiments in the following chapter.
CHAPTER 3

NUMERICAL VALIDATION OF VCFEM FOR UNDAMAGED HETEROGENEOUS MEDIA

3.1 Introduction

In this chapter the effectiveness of VCFEM to model deformations in heterogeneous media is presented. VCFEM is compared with numerical simulations using traditional displacement based finite element methods as well as with published results in the literature. A more detailed set of simulations for undamaged random heterogeneous media consisting of voids/inclusions can be found in [55, 56].

Representative material elements (RME) characterize a microstructure at a given point in a structure. Material properties of macroscopic points of the structure correspond to the volume average of the microscopic response and are referred to as the macroscopic response of the RME. In particular, macroscopic stress components $\bar{\sigma}_{ij}$ are obtained from the true microscopic stresses $\sigma_{ij}$ following the relation

$$\bar{\sigma}_{ij} = \frac{1}{V_{RME}} \int_{a_{RME}} \sigma_{ij} dV,$$

where $V_{RME}$ is the volume of the representative material element. Correspondingly, the macroscopic strains are given as

$$\bar{\varepsilon}_{ij} = \frac{1}{V_{RME}} \int_{a_{RME}} \varepsilon_{ij} dV.$$
In order for an RME to effectively characterize material properties at a macroscopic point it is assumed that the material morphology repeats itself in a small neighborhood of that point. Such an assumption can be thought of as homogeneous deformations across the boundaries of the RME and are referred to as repeatability conditions. Thus for the RME shown in figure (3.1), the surface \( x = L \) has to remain straight so that its deformations are similar to its adjacent surface \( x = 0 \). Mathematically such a condition is enforced as, \( \Delta u_x = \Delta \bar{u} \) on \( x = L \) such that the average internal traction on this surface \( \int_{x=L} t_x dS = 0 \). The average traction requirement is enforced in a weak sense, and consequently the unknown displacement \( \Delta \bar{u} \) is evaluated naturally as part of the VCFE solution.

3.2 Comparison of VCFEM and ABAQUS for Square Edge Packed RME with Circular Inclusions

Representative material elements consisting of square edge packed heterogeneities, loaded in simple tension are considered in this example. Figure (3.2) depicts the RME with a square edge packed circular inclusion and its associated loading conditions. Material properties of the constituents are as follows:

**Al-3.5% Cu Matrix**

Young’s Modulus \( E = 72 \) GPa, Poisson’s Ratio \( \nu = 0.32 \)

Post yield behavior (Power law hardening) \( \sigma_m = \sigma_0 (\epsilon_m^p/\epsilon_0 + 1)^N \), where the initial flow stress is \( \sigma_0 = 175 \) MPa, the strain hardening exponent is \( N = 0.2 \), and \( \epsilon_0 = \sigma_0/E \) is the uniaxial strain at yield.

**SiC Inclusions**

Young’s Modulus \( E = 450 \) GPa, Poisson’s Ratio \( \nu = 0.17 \)
Figure 3.1: Periodic morphology at a macroscopic point and the representative material element (RME) depicting the microstructure

Figure 3.2: Schematic for a RME with a $V_f = 20\%$ square edge packed circular inclusion
Figure 3.3: (a) VCFEM and (b) ABAQUS meshes for RME with a $V_f = 20\%$ square edge packed circular inclusion

Figure 3.4: Macroscopic stress-strain response for RME with $V_f = 20\%$ square edge packed circular inclusions
Figure 3.5: Microscopic tensile stress distribution for RME with $V_f = 20\%$ square edge packed circular inclusions at a macroscopic tensile strain of $\varepsilon_{yy} = 1\%$ along (a) $y/R=0$ (b) $y/R=1/3$ (c) $y/R=2/3$ and (d) $y/R=1$
Repeatability conditions are enforced on the free surface \( x = L/2 \) and the RME is loaded incrementally to a maximum macroscopic tensile strain of \( \varepsilon_{yy} = 1\% \) under plane strain conditions. VCFEM and ABAQUS meshes used to analyze the problem are shown respectively in figures (3.3a and b). VCFEM mesh consists of 1 element with its outer boundary discretized through 12 node (nodes are marked with a “x”) into linear elements. The inclusion boundary is discretized through 8 nodes into quadratic line elements in order to reflect its curvature. The matrix stress in this problem is represented using a 6th order polynomial airy stress function contributing 25 \( \beta \) parameters \((p + q = 2..4)\) to the stress interpolation. 3 reciprocal terms for each 2nd order polynomial terms \((i = p + q..p + q + 2 \forall p + q = 2)\) contributing 9 \( \beta \) parameters in the stress interpolation are used to simulate shape effects of the circular inclusions. The reciprocal function \( f \) is generated using the conformal mapping of the circular inclusions \((f = r/R)\). Quarter symmetry has been invoked in the ABAQUS mesh which consists of 455 QUAD4 elements discretized through 471 nodes. Figure (3.4) shows the resulting macroscopic stress-strain response. These plots show an show excellent agreement between the VCFEM and ABAQUS results. Figure (3.5a, b, c and d) shows a comparison of the microscopic tensile stress distribution along the 4 sections passing through the inclusion at a macroscopic tensile strain of \( \varepsilon_{yy} = 1\% \). VCFE results are in good agreement with ABAQUS, with slight discrepancies noticed at the matrix-inclusion interface. These results demonstrate the effectiveness of VCFEM to model both microscopic and macroscopic response of simple microstructures.
Figure 3.6: (a) VCFEM and (b) ANSYS meshes for RME with $V_f = 20\%$ random packed circular inclusions

Figure 3.7: Histograms for quantitative characterization of the random packing composite ($V_f = 20\%$). Frequency of occurrence of (a) Area ratio (b) Mean neighbor distance
3.3 Comparison of VCFEM and ANSYS for Randomly Packed RME with Circular Inclusions

In this example, a microstructural RME with 29 randomly distributed circular boron fibers, with a volume fraction $V_f = 20\%$, in a 6061-O Al matrix is analyzed. Figure (3.6a and b) shows the discretization employed by VCFEM and ANSYS models. The ANSYS mesh consists of 8000 QUAD4 elements, while the VCFEM mesh has only 29 elements corresponding to the number of inclusions. The locations of these inclusions were generated by a random number generator suggested in [61]. Histograms in figures (3.7a and b) indicate morphological features obtained through quantitative characterization for this microstructure. Material properties of the constituents are as follows:

**6061-O Al Matrix**

Young's Modulus $E = 69$ GPa, Poisson's Ratio $\nu = 0.33$

Post yield behavior (Power law hardening) $\sigma_m = \sigma_0^0 + 0.14 \times \varepsilon_m^{0.333} \text{ GPa}$ where the initial flow stress $\sigma_0 = 43$ MPa, and the effective stress and strain in the matrix are denoted respectively by $\sigma_m$ and $\varepsilon_m$

**Boron Fibers**

Young’s Modulus $E = 410$ GPa, Poisson’s Ratio $\nu = 0.2$

The RME is loaded incrementally under plane strain conditions to a maximum macroscopic tensile strain of $\varepsilon_{xx} = 0.5\%$. As in the previous example, the matrix stress function consists of 25 polynomial terms and 9 reciprocal terms, while the inclusion stress function has the 25 polynomial terms. Figure (3.8) shows the overall macroscopic tensile stress-strain response by the two methods. A near perfect match is obtained for all stages of the loading curve. Figure (3.9) shows the true microscopic
Figure 3.8: Macroscopic stress-strain response for RME with $V_f = 20\%$ random packed circular inclusions

Figure 3.9: Microscopic Tensile Stress Distribution for RME with $V_f = 20\%$ Random Packed Circular Inclusions at a Macroscopic Tensile Strain of $\bar{e}_{xx} = 0.5\%$ along (a) $x/R=0.4$ (b) $x/R=0.7$
stress distribution at two different sections (x/L=0.4 and x/L=0.7). While the stress distributions by the two methods are in good agreement, small discrepancies in peak stresses inside the inclusions and and across Voronoi cell boundaries. The example illustrates the effectiveness of VCFEM for modeling severely fluctuating deformation fields in random heterogeneous microstructures.

3.4 Validation of VCFEM for Square Diagonal Packed RME with Square Shaped Inclusions

In the next example, results obtained by VCFEM are compared with those generated by Finot et.al[47] and the software package ABAQUS. The example also provides a simple analysis of mesh/stress interpolation dependencies of the VCFEM. Square diagonal packed representative material elements (RME) composed of square shaped
Figure 3.11: Distribution of the maximum principal stress generated by (a) ABAQUS and (b) Finot et al. [1] for RME with square shaped inclusions. Results are scaled to the matrix yield strength $\sigma_0$.

Inclusions used in the simulation is shown in figure (3.10). The volume fraction of the inclusions are $V_f = 20\%$ and periodicity conditions are enforced on the free surface ($x = L$). The analysis is carried out under plain strain conditions. Material properties of the constituents are as follows:

**Al-3.5% Cu Matrix**

Young’s Modulus $E = 72$ GPa, Poisson’s Ratio $\nu = 0.32$

Post yield behavior (Power law hardening) $\sigma_m = \sigma_0(e_m^p/\epsilon_0 + 1)^N$,

where the initial flow stress $\sigma_0 = 175$ MPa, the strain hardening exponent $N = 0.2$, and $\epsilon_0 = \sigma_0/E$ is the uniaxial strain at yield.

**SiC Inclusions**
Young’s Modulus $E = 450$ GPa, Poisson’s Ratio $\nu = 0.17$

In order to effectively simulate the distribution using the VCFEM, it is essential to model both the displacement and stress fields near the vertex of the inclusions accurately. Consequently, in all of the VCFE meshes considered in this example (see figure 3.12a, b, and c), each of the square shaped inclusions are modeled using 10 nodes. Two nodes near the corner of the squares are used to better represent the rapidly fluctuating displacement field near the vertex of the inclusion. The ABAQUS mesh (not shown) consists of 1600 square shaped QUAD4 elements. Figure (3.11a and b) depict the distribution of the maximum principal stress at the end of the loading generated respectively by ABAQUS and Finot et.al. The results shown in the figure have been scaled to matrix yield strength $\sigma_0$. The contour plots depict a bigger gradient in the stress field for the regions in and around the larger inclusion. The largest stress gradients at the corners of the inclusions are due to presence of the reentrant corner at the square vertices. The effect of discretization of the RME and the stress representations in the Voronoi cells are studied in the following sections.

3.4.1 Effect of discretization

Figures (3.12a, b and c) show the 3 VCFE meshes used to study the effect of discretization on the deformation the RME. The first mesh was produced by the Dirichlet tessellation of the RME. In the second mesh, the side (the diagonal of the RME) representing points equidistant from the surfaces of the adjacent inclusions is replaced by a vertical side. In the last mesh, the RME is discretized into 4 VCFEs,
Figure 3.12: Three VCFE meshes used to study the effect of discretization on the deformation of the RME with square shaped inclusions.

Figure 3.13: Distribution of maximum principal stress generated for the three VCFE meshes with square shaped inclusions. Results are scaled to the matrix yield strength $\sigma_0$. 

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two of which contain the square inclusions. In each of the RMEs', elements containing
inclusions are modeled using a 61 term stress function generated using 25 polynomial
terms (6th order complete polynomial expansion of the Airy function, i.e. \( p+q = 2..6 \))
and and 36 reciprocal terms (3 reciprocal terms for each polynomial exponent from
2 to 4, i.e. \( i = p + q..p + q + 2 \ \forall \ p + q \in [2,4] \)), while elements containing no
inclusions are modeled using only the first 25 polynomial terms. A 20 term fourier
expansion was used to generate the shape of the inclusions and the displacement
field on the voronoi cell and inclusion boundaries are modeled using linear shape
functions between the nodes. The resulting maximum principal stress distribution in
the RME at the end of the loading is shown in figure (3.13a, b and c). The contour
plots for the first two VCFE meshes are in excellent agreement with those generated
by ABAQUS and Finot et.al. Cutoff values produced in the matrix are identical
with those generated by ABAQUS and Finot et.al., while the contours generated
in the matrix match very well with those generated by ABAQUS. Deviations from
simulations by Finot et.al. can be seen over areas at the left and right corners of the
RME, while deviations from the ABAQUS simulations are visible near the vertex of
the inclusion. Minor differences between the matrix stress distributions for the two
VCFE meshes can be seen nearer the larger inclusions. Within the inclusions, the
principal stress distribution match reasonably well with both ABAQUS and Finot
et.al. While the ABAQUS results depict a sharp gradient in stress field near the
corner, the VCFE results depict a more gradual distribution in the stress field near the
corners. A value of around 2.3 generated by VCFEM, at the edges of the inclusions,
is in very good agreement with Finot’s results. The corresponding value generated by
AB AQUS is around 5.16. Deviations between VCFEM and traditional FEMs near
the vertex of the inclusions are attributed to the smoothened nature of the fourier expansion which has been used to simulate the sharp corner. It should be noted here that the alternative discretizations to the Dirichlet tessellation, like those used in figure (3.12b) maybe much more difficult to generate in the random RME case. However, the last mesh produces a stress field that sharply deviates from simulations by ABAQUS and Finot et.al. The differences produced are attributed to the simplified stress field used for the 2 elements without the inclusions. Such elements produce very little error when the stress distribution is fairly uniform (as is the element to the right), but produce significantly different stress distributions if they are in regions with varied stress distributions (as is the element to the top). However in a random RME which is loaded arbitrarily, the uniformity of the stress field in specified regions cannot be predetermined and hence the discretization employed in figure (3.13c) is not recommended.

3.4.2 Effect of fourier expansion and stress functions

In order to study the effectiveness of the shape functions used, two examples are considered in this section. In the first example, the shape of the inclusion is represented using a 10 term fourier series and the VCFE mesh used in figure (3.12a) is analyzed. The resulting principal stress distribution at the end of the loading is shown in figure (3.14a). The results show that regions close to the inclusion (especially close to the sharp corner) are somewhat smoothened. Such an effect is to be expected, since the 10 term fourier expansion produces a much smoother representation near the vertex of the square inclusion. In the next example, a 34 term expansion for the
Figure 3.14: Distribution of the maximum principal stress in RME with square shaped inclusions generated by (a) 10 term fourier expansion for the square boundary of the inclusions (b) 34 term stress function in the matrix of the voronoi cells. The results are scaled to the matrix yield strength $\sigma_0$.

airy function $p + q = 2.6$ and $i = 1.3Vp + q = 2$) is used to represent the stress field in matrix of the VCFEs in figure (3.12a). The resulting distribution of the maximum principal stresses at the end of the loading is shown in figure (3.14b). While the principal stresses around the smaller inclusion are well represented by the new stress function, the stresses along the edge of the larger inclusion show a larger discrepancy. This effect is attributed to the fact that as the inclusion becomes larger and hence approach the Voronoi cell boundary, polynomial stresses of higher orders $p + q > 2$ need to be neutralized by reciprocal stress functions. We can thus conclude, that for square inclusions a 20 term fourier expansion coupled with a 61 term stress function can be used to effectively model voronoi cells in the RME. The VCFEM is also shown to be mesh sensitive, especially when parts of the RME are represented by simpler
polynomial stress fields. It is also important to predetermine the required level of accuracies for the displacement field at the boundaries based on the shape of the inclusions.

3.5 A Square Homogeneous Domain with an Elliptical Crack

While the primary focus of this work is to model damage in non-linear random heterogeneous media, a considerable number of results in the literature are available for damaged non-linear homogeneous media. One such result is compared with the VCFEM in this example. The RME consisting of square edge packed elliptical cracks in a hardening matrix is shown in figure (3.15a). VCFEM is compared to the Hutchinson-Rice-Rosengren [81] (HRR) field generated using an asymptotic analysis of a sharp crack in a non-linear elastic matrix. The elliptical crack has an aspect ratio of $a/b = 100$ and the RME has a dimension of $a/L = \frac{1}{10}$. Material properties are as follows:

Matrix Material

Young’s Modulus $E = 50$ units, Poisson’s Ratio $\nu = 0.33$

Post yield behavior (Ramberg-Osgood law) $\sigma_m = \sigma_0 \left( \frac{\epsilon}{\epsilon_0} \right)^{1/n}$,

where the initial flow stress of the matrix $\sigma_0 = 1$ unit, $\epsilon_0$ is the strain at yield ($\epsilon_0 = \frac{a_0}{E}$), and the material parameter $\alpha = 0.02$. The strain hardening exponents of $n = 3$ and $n = 13$ are considered in the example.
Figure 3.15: (a) Schematic for the RME with an elliptical crack (b) VCFE mesh used to analyze the problem in (a)

The RME is loaded in uniaxial tension perpendicular to the face of the crack to a macroscopic tensile strain $\varepsilon_{yy} = 0.5\%$. The VCFE mesh used in the analysis is shown in figure (3.15b). The element boundary is discretized using 8 nodes (nodes are marked with a "x" in the figure) with linear displacement interpolation between the nodes. The elliptical crack is modeled using 8 nodes, with the curvature of the crack realized using quadratic line elements between the nodes. The matrix stress function consists of 12 polynomial terms (4-th order polynomial Airy function, i.e. $p + q = 2..4$) and 36 reciprocal terms based on the conformal function for the elliptical crack (3 reciprocal terms for each polynomial exponent from 2 to 4, i.e. $i = p + q..p + q + 2 \forall p + q \in [2,4]$). The analysis is carried out under both plane stress and plane strain conditions.
Sanders[82] and Rice[83] have proposed that under the assumptions of small scale yielding the elastic-plastic $J$ integral for contours far removed from the crack-tip have the same values as their linear elastic counterparts. Formally, the linear elastic $J$ integral for finite crack sizes is given as [82], $J_{\text{PlaneStress}} = \frac{\bar{\sigma}_{yy}^2}{E} \frac{R_s}{L} \tan \frac{R_s}{L}$ and $J_{\text{PlaneStrain}} = (1 - \nu^2)J_{\text{PlaneStress}}$ where $\bar{\sigma}_{yy}$ is the far field macroscopic stress. The variations of the $J$ integral with macroscopic loading under plane strain and plane stress conditions are shown respectively in figures (3.16a and b) for strain hardening exponents of $n = 1, 3$ and 13. VCFE results are in excellent agreement to the theoretical values (a maximum error of 2% for either case) upto a macroscopic load of $\bar{\sigma}_{yy} = 0.14 \sigma_0$. At higher macroscopic load levels, the VCFE depicts higher values for $J$ integrals indicating a departure from small scale yielding solution.
Figure 3.17: Variation of (a) cylindrical stress components with radial distance at \( \theta = 0 \) and (b) effective stress with the polar angle at \( r/b = 1 \) for a hardening exponent \( n = 3 \), plane stress calculations.

The asymptotic HRR field predicts that at a constant angle \( \theta \) (see figure 3.15) the individual components of the stresses vary as

\[
s_{ij} = \frac{K}{r^{s}}\hat{\sigma}_{ij}(\theta), \quad s = \frac{1}{n+1}
\]

Figure 3.17a) show the variation of the microscale stresses at an angle \( \theta = 0 \) for a strain hardening exponent \( n = 3 \) under plane stress conditions as a function of the radial distance. The HRR field predictions are plotted by equating the VCFEM stresses at \( \xi = 10 \) to that in equation (3.1) for evaluating \( K\hat{\sigma}_{ij}(\theta)|_{\theta=0} \). These results show excellent correlation with the HRR field until near the crack tip \( (r/b = 1.0) \). For lower radial distances, the stress component \( \sigma_{rr} \) begins to drop. The decrease in radial component of the stress is because the traction \( t_r = \sigma_{rr} \) at the tip of the elliptical crack vanishes to satisfy zero traction boundary conditions at \( r/b = 0 \). The
Figure 3.18: (a) Variation of cylindrical shear stress component $\sigma_{r\theta}$ with the polar angle at $r/b = 1$ and (b) Effective plastic strain (%) at the crack tip for hardening exponent $n = 3$, plane stress calculations.

drop in the radial component $\sigma_{rr}$ triggers a fall in the hoop component $\sigma_{\theta\theta}$ at a radial distance $r/b = 0.2$. These results are in qualitative agreement with finite element calculations by McMeeking [85] for blunt cracks. The angular variation of the Von Mises stress $\sigma_m$ and shear stress $\sigma_{r\theta}$ at $r/b = 3$ are compared with the HRR field in figure (3.17b and 3.18a) respectively. The plots are in good agreement with their respective HRR counterparts up to an angle of $\theta = 90^0$. However for $\theta > 90^0$, there is a deviation from HRR results. This may be attributed to the blunt nature of the elliptical crack, since radial lines intersect the elliptical crack on the blunt surface where zero traction boundary conditions exist on the crack surface. Finally the effective plastic strain distribution in a small region ($10b \times 8b$ window) near the crack tip is shown in figure (3.18b). It can be seen from this plot that the plastic straining
extends ahead of the crack tip for the plane stress case. Similar observations have been made by Hutchinson [81] and Rice [83].

3.6 Conclusions

In this chapter, the effectiveness of VCFEM to model 2-dimensional elasto-plastic deformations in undamaged heterogeneous media has been presented. Microstructures with both voids/inclusions of various shapes and morphologies have been analyzed. Results indicate that the VCFEM provides an accurate representation of the deformation in such materials at both macroscopic and microscopic levels. Examples studied provide the required stress interpolation functions for RMEs with inclusions and voids, and there effectiveness in analyzing deformations with various discretizations. In the next chapter, VCFEM is extended to model damage in random heterogeneous materials.
CHAPTER 4

VORONOI CELL FINITE ELEMENT METHOD FOR DAMAGED RANDOM HETEROGENEOUS MEDIA

4.1 Introduction

Metal matrix composites such as Al, Ti and Ni alloys reinforced with $Al_2O_3$ or $SiC$ inclusions considerably enhance flow strength and toughness at ambient temperature as well as provide adequate creep resistance at elevated temperature. An important feature of these composites is that the reinforcements are brittle, contain defects such as microcracks and the particle/matrix interface may contain initial flaws. Overall tensile loading can consequently lead to particle cracking and interface decohesion. Such phenomena can cause considerable drop in the composite flow strength and creep resistance and ultimately lead to catastrophic failure of the material. A proper understanding of the deformation processes involved in the failure of random microstructure can therefore prove indispensable in the design of such composites.

VCFEM developed in the previous chapters for modeling undamaged heterogeneous media is extended in this chapter to model damage in such materials. Failure in the microstructure is modeled in the form of abrupt particle cracking/splitting triggered by a maximum principle stress or Rankine theory. The distinction between
Figure 4.1: (a) Representative material element (b) Voronoi cell finite element with cracked particle

complete particle cracking and splitting is made through the assumption, that in the former case the tip of the crack is still in the particle, while in the latter case, the tip has just moved into the matrix. Complete particle cracking and splitting is assumed at the onset of damage evolution, thereby avoiding the problem of crack propagation within each inclusion. Justification of this assumption is derived from the fact that (a) for the multitude of inclusions considered, crack propagation in each inclusion would make the problem inordinately large and (b) experimental observations imply very quick transition from particle crack initiation to splitting. The resulting element thus consists of three phases, viz. the matrix phase, the inclusion phase and the crack phase which is represented as an elliptical void with a high aspect ratio ($\sim 10 -100$). The energy functional (2.2) is thereby modified to accommodate the new topology
introduced into the Voronoi cell. The resulting weak form of the variational principle, finite element equations and numerical aspects of the computational method are also presented. Physical motivation to determine the critical stress to failure of individual particles in actual mesostructures is also discussed. VCFEM development for undamaged media, presented in Chapter 2, extend naturally into this chapter and are therefore used as a starting point in the discussions that follow.

4.2 Assumed Stress Hybrid Variational Principle for Damaged Voronoi Cells

Consider a RME consisting of \( N \) voronoi cells consisting both damaged/undamaged elements with a typical BSE consisting of a damaged inclusion as shown in figures (4.1 a and b). In addition to the displacement/stress fields outlined in section 2.3, the displacement field on the crack boundary \( \partial \Omega_{cr} \) at the beginning of and during the \( p \)th increment are respectively taken to be \( \Delta u'' \) and \( \Delta u'' \). The energy functional (2.2) is thereby modified to accommodate the third phase as:

\[
\Pi_{e}^{C}(\Delta \sigma, \Delta u) = - \int_{\Omega_{e}} \Delta B(\sigma, \Delta \sigma) \, d\Omega - \int_{\Omega_{e}} e : \Delta \sigma \, d\Omega - \int_{\partial \Omega_{e}} (\sigma + \Delta \sigma) \cdot n^{e} \cdot (u + \Delta u) \, d\Gamma
\]
\[- \int_{\partial \Omega_{e}} \left( \sigma^{m} + \Delta \sigma^{m} - \sigma^{c} - \Delta \sigma^{c} \right) \cdot n^{e} \cdot (u' + \Delta u') \, d\partial \Omega
\]
\[- \int_{\partial \Omega_{cr}} (\sigma^{c} + \Delta \sigma^{c}) \cdot n^{c} \cdot (u'' + \Delta u'') \, d\partial \Omega \quad (4.1)
\]

with the global energy functional given by

\[
\Pi^{C} = \sum_{e=1}^{N} \Pi_{e}^{C} \quad (4.2)
\]
In equation (4.1), superscript \( cr \) corresponds to variables on the crack boundary and \( n^{cr} \) the outward normal on the crack face. The first variation of \( \Pi^C \) and \( \Pi^C \) with respect to its arguments, yield all relations in euler equations (2.3, 2.4, 2.5 and 2.6) and additionally the zero traction condition on the crack boundary \( \partial \Omega_{cr} \).

\[
(\sigma^c + \Delta \sigma^c) \cdot n^{cr} = 0 \text{ on Interface } \partial \Omega_{cr}
\]  

Equilibrated stress increments \( \Delta \sigma \), constitutive relations and euler equations (2.3, 2.4, 2.5, 2.6 and 4.3) completely define the new microstructural problem at the \( p \)th increment.

4.3 Element Formulations and assumptions

4.3.1 Crack enhanced stress functions for damaged voronoi cells

With the addition of an extra phase in the form of a blunt crack, the stress functions and their associated fields expressed in equations (2.39, 2.38 and 2.7) are automatically adjusted to account for the altered topology. In this procedure, the crack boundary \( \partial \Omega_{cr} \) is parametrically represented through a conformal mapping technique as a function \( f_{cr}(x, y) = 1 \), similar to equation (2.11). The mapped function \( f_{cr} \) represents a specialized radial coordinate which depend on the shape of the ellipse and exhibits the property that \( f_{cr} \rightarrow \infty \) as \((x, y)\rightarrow \infty\). The Airy's stress functions for the matrix and inclusion phases are constructed by superposing reciprocal terms derived from the conformal mapping function \( f_{cr} \) of the crack boundary:

\[
\Phi^m = \Phi_{poly}^m + \Phi_{rec}^m + \Phi_{rec}^{cm}
\]
\[
\Phi^c = \Phi_{poly}^c + \Phi_{rec}^{cc}
\]
where the contributions $\Phi_{\text{rec}}^{\text{cm}}$ and $\Phi_{\text{rec}}^{\text{cc}}$ due to the crack is written as:

\[
\Phi_{\text{rec}}^{\text{cm}} = \sum_{p,q} \xi^p \eta^q \sum_{i=1}^{n'} \left( \frac{\Delta \beta_{\text{pq}i}}{f_{\text{cr}}^{p+q+i-1}} \right)
\]
\[
\Phi_{\text{rec}}^{\text{cc}} = \sum_{p,q} \xi^p \eta^q \sum_{i=1}^{n'} \left( \frac{\Delta \beta_{\text{pq}i}}{f_{\text{cr}}^{p+q+i-1}} \right)
\]  \hspace{1cm} (4.5)

While the reciprocal terms $\frac{1}{f_{\text{cr}}^{p+q+i-1}}$ in $\Phi_{\text{rec}}^{\text{cc}}$ facilitate traction boundary conditions on the crack boundary $\partial \Omega_{\text{cr}}$, they provide asymptotic stress gradients, through $\Phi_{\text{rec}}^{\text{cm}}$, for matrix material near the crack tip. Stresses are obtained by taking derivatives of the Airy stress functions as:

\[
\begin{align*}
\Delta \sigma_{xx} & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{cm}}}{\partial x^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{cc}}}{\partial y^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial x \partial y} \Delta \beta_{pq} \right\} \\
\Delta \sigma_{yy} & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{cm}}}{\partial y^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{cc}}}{\partial x^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial y \partial x} \Delta \beta_{pq} \right\} \\
\Delta \sigma_{xy} & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial x \partial y} \Delta \beta_{pq} \right\} \\
\end{align*}
\]

\[
\begin{align*}
\Delta \sigma_{xx}^c & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{cm}}}{\partial x^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{cc}}}{\partial y^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial x \partial y} \Delta \beta_{pq} \right\} \\
\Delta \sigma_{yy}^c & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{cm}}}{\partial y^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{cc}}}{\partial x^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial y \partial x} \Delta \beta_{pq} \right\} \\
\Delta \sigma_{xy}^c & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial x \partial y} \Delta \beta_{pq} \right\} \\
\end{align*}
\]

\[
\begin{align*}
\Delta \sigma_{xx}^c & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{cm}}}{\partial x^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{cc}}}{\partial y^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial x \partial y} \Delta \beta_{pq} \right\} \\
\Delta \sigma_{yy}^c & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{cm}}}{\partial y^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{cc}}}{\partial x^2} \Delta \beta_{pq} + \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial y \partial x} \Delta \beta_{pq} \right\} \\
\Delta \sigma_{xy}^c & = \left\{ \frac{\partial^2 \Phi_{\text{rec}}^{\text{mc}}}{\partial x \partial y} \Delta \beta_{pq} \right\} \\
\end{align*}
\]  \hspace{1cm} (4.6)

4.3.2 Displacement field on the crack surface

In addition to the displacement field interpolation $\Delta u$ and $\Delta u'$ used in equations (2.19), the displacement field $\Delta u''$ is interpolated from the corresponding values $\{\Delta q''\}$ at the nodes on the crack surface as:

\[
\{\Delta u''\} = [L^c]\{\Delta q''\}
\]
In order to realize an elliptical crack geometry, points on the crack surface \((x_{cr}, y_{cr})\) are obtained through a quadratic interpolation of nodal values as:

\[
x_{cr} = 2(1 - a/l_i)(1/2 - a/l_i)x_i + (1 - a/l_i)a/l_i x_m + 2a/l_i(a/l_i - 1/2)x_{i+1}
\]
\[
y_{cr} = 2(1 - a/l_i)(1/2 - a/l_i)y_i + (1 - a/l_i)a/l_i y_m + 2a/l_i(a/l_i - 1/2)y_{i+1}
\]

where \((x_i, y_i)\) and \((x_{i+1}, y_{i+1})\) are respectively the cartesian coordinates of adjacent nodes \(i\) and \(i + 1\), \(l_i\) is the curvilinear distance between them, \(a\) is the curvilinear distance between \((x_{cr}, y_{cr})\) and node \(i\) and \((x_m, y_m)\) are coordinates of the mid-node (i.e. \(a_m = l_i/2\)). While the above representation of the crack surface does not directly contribute to the linear interpolation matrix \([L^e]\) (which is the similar to \([L^c]\) in equation 2.19), they provide accurate curvilinear contributions to the jacobian \(d\Omega\) used in the calculation of the \([G^e]\) in section 4.4.

### 4.3.3 Weak form of the assumed stress hybrid variational

Substituting element approximations for stresses (4.6) and displacements (2.19 and 4.3.2) in the energy functional (4.1), and setting the first variations with respect to the stress parameters \(\Delta \beta^m\) and \(\Delta \beta^c\) respectively to zero, results in the following two weak forms of the kinematic relations (2.3),

\[
\int_{\Omega_e} [P^m]^T \{\epsilon + \Delta \epsilon\} d\Omega = \int_{\Gamma_e} [P^m]^T [n^e] [L^e] d\Gamma \{\Delta q\} - \int_{\Gamma_e} [P^m]^T [n^e] [L^e] d\Gamma \{\Delta q'\}
\]
\[
\int_{\Omega_c} [P^c]^T \{\epsilon + \Delta \epsilon\} d\Omega = \int_{\Gamma_c} [P^c]^T [n^e] [L^c] d\Omega - \int_{\Gamma_c} [P^c]^T [n^e] [L^c] d\Omega \{\Delta q''\} \quad (4.7)
\]

Furthermore, setting the first variation of the total energy functional in equation (2.2) with respect to increments in nodal displacements \(\Delta q\), \(\Delta q'\) and \(\Delta q''\), result in the weak form of the traction reciprocity conditions

\[
\sum_{e=1}^{N} \begin{bmatrix}
\int_{\Gamma_e} [L^e]^T [n^e]^T [P^m] d\Omega & 0 \\
0 & \int_{\Gamma_{cr}} [L^{cr}]^T [n^{cr}]^T [P^c] d\Omega
\end{bmatrix}
\begin{bmatrix}
\beta^m + \Delta \beta^m \\
\beta^c + \Delta \beta^c
\end{bmatrix} = \begin{bmatrix}
0 \\
0
\end{bmatrix}
\]

67
Equations (4.7 and 4.8) along with the constitutive relations developed in section 2.4 can now be used to solve for the unknown stress coefficients and nodal displacements.

4.4 Solution Method for the Weak Form

An iterative solution process is invoked for equation (4.7) to evaluate the stresses, given the nodal displacement increments \( \{ \Delta q \} \) \( \{ \Delta q' \} \) and \( \{ \Delta q'' \} \). Let \( \{ \delta \beta \}^i \) correspond to the correction to the value of \( \Delta \beta \) in the \( i \)-th iteration, i.e.

\[
\{ \Delta \beta^m \} = \{ \Delta \beta^m \}^i + \{ \delta \beta^m \}^i
\]

\[
\{ \Delta \beta^c \} = \{ \Delta \beta^c \}^i + \{ \delta \beta^c \}^i
\]

The kinematic equation (4.7) may then be linearized with respect to \( \Delta \beta \) to yield:

\[
\begin{bmatrix}
H_m & 0 \\
0 & H_c
\end{bmatrix}
\begin{bmatrix}
\Delta \beta^m \\
\Delta \beta^c
\end{bmatrix}
^i
=
\begin{bmatrix}
G_e & -G_{cm} & 0 \\
0 & G_{cc} & -G_{cr}
\end{bmatrix}
\begin{bmatrix}
q + \Delta q \\
q' + \Delta q' \\
q'' + \Delta q''
\end{bmatrix}
-
\begin{bmatrix}
\sum_{t=1}^N [L^e]^T \{ \dot{t} + \Delta t \} d\Omega \\
\sum_{t=1}^N [L^e]^T \{ \dot{t} + \Delta t \} d\Omega
\end{bmatrix}
\]

In a condensed form this can be restated as:

\[
[H] \{ \delta \beta \}^i = [G] \{ \Delta u \} - \left\{ \sum_{t=1}^N [P^m]^T \{ \epsilon + \Delta \epsilon \}_i^t d\Omega \right\} \forall \ e = 1 \cdots N \quad (4.10)
\]

where matrices \([H_m], [H_c], [G_e], [G_{cm}], \) and \([G_{cc}]\) are obtained from equation (2.35), \([S(x, y)]\) is the instantaneous elastic-plastic tangent compliance tensor as derived in equation (2.31) and

\[
[G_{cr}] = \int_{\partial \Omega_{cr}} [P^c]^T [n^\sigma] [L^\sigma] d\Omega \quad (4.11)
\]
As in the undamaged case, the linearized matrix equation (4.10) is solved for the stress function coefficients using a Quasi-Newton iterative solution procedure [75].

Proceeding in the same way as for stresses, let \( \{ dq \}^j \) correspond to the correction in \( \{ \Delta q \} \) in the \( j \)-th iteration of (4.8), i.e.

\[
\{ \Delta q \} = \{ \Delta q \}^j + \{ dq \}^j
\]

\[
\{ \Delta q' \} = \{ \Delta q' \}^j + \{ dq' \}^j
\]

\[
\{ \Delta q'' \} = \{ \Delta q'' \}^j + \{ dq'' \}^j
\]

\( (4.12) \)

Substituting equation (4.10) in the linearized weak form of the global traction reciprocity equation (4.8) and taking variations with respect to the displacement increment \( \{ \Delta q \} \), yields the following matrix equation:

\[
\sum_{e=1}^{N} \left[ G^T \right]^{-1} \left[ H \right] \begin{bmatrix} \frac{d\mathbf{q}}{d\mathbf{q}'} \frac{d\mathbf{q}''}{d\mathbf{q}''} \end{bmatrix}^j = \sum_{e=1}^{N} \left\{ \begin{bmatrix} f_{r_m}[L^m]^T \{ \mathbf{t} + \Delta \mathbf{t} \} & d\Omega \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} f_{\beta_m}[L^c]^T \{ \mathbf{n}^m \}^T & 0 \\ -f_{\beta_c}[L^c]^T \{ \mathbf{n}^m \}^T^T \{ \mathbf{P}^m \}^T & d\Omega \end{bmatrix} \right\}^j \begin{bmatrix} \mathbf{\beta}^m + \Delta \mathbf{\beta}^m \\ \mathbf{\beta}^c + \Delta \mathbf{\beta}^c \end{bmatrix}
\]

or, in standard finite element notation

\[
\sum_{e=1}^{N} \left[ \mathbf{K}_e \right] \{ d\mathbf{u} \}^j = \sum_{e=1}^{N} \{ f_e \}^j
\]

\( (4.13) \)

The linearized global traction reciprocity condition in equation (4.13) is used to iteratively solve the traction reciprocity condition (4.8) for the nodal displacement increments.
4.5 Numerical Aspects of VCFEM for Damaged Heterogeneous Media

As for the undamaged Voronoi cells, effective implementations of VCFEM demands rigid control on the numerical stability of the various matrix systems developed in the previous sections. Numerical techniques developed in section 2.6 for proper conditioning of matrices $[H_m]$ and $[H_c]$, optimal choice of stress coefficients, and suppression of rigid body modes on the inclusion interface are essentially carried over to the implementation stage of VCFEM for damaged media. However, the introduction of a new topology onto the Voronoi cell requires a modified integration procedure in the matrix and inclusion domains of the Voronoi cell. These are presented next.
4.5.1 Numerical integration of element matrices in the two phases of the Voronoi cell

With the introduction of the crack surface into the Voronoi cell, two essential features are incorporated in the discretization procedure discussed in section 2.6.2. Firstly, for damaged voronoi cells sharpest stress gradients arise from reciprocal terms \( \frac{1}{f_{cr}} \). Consequently the mapping function \( f_{cr} \) of the crack boundary is used as the driving force in the discretization of the matrix domain. Secondly, the inclusion domain no longer remains simply connected and hence its subdivision into triangles is no longer feasible. The inclusion domain with a crack boundary can be visualized like a the matrix domain with an inclusion boundary. Thus the subdivision of the inclusion domain into quadrilaterals is implemented using the algorithm developed for the matrix domain in section 2.6.2. These two features have been incorporated into a damaged voronoi cell in figure (4.2). The first feature results in a concentration of quadrilaterals (and therefore integration points) near the crack tip of the matrix domain. This in turn leads to an efficient representation of the asymptotic fields at the crack tip. The second feature results in the subdivision of the damaged particle into quadrilaterals that provide for accurate integration of the reciprocal stress functions in the inclusion domain.

4.6 Fracture Mechanics Based Damage Criterion

The inclusion in this thesis is assumed to be brittle and is consequently modeled as an elastic material. Microstructural damage in the inclusion by particle cracking and splitting is initiated by a maximum principal stress theory, also known as the
Rankine criterion. In this criterion, a crack is initiated once the maximum tensile principal stress exceeds a critical failure stress $\sigma_{cr}$. In the computational procedure, once the principal tensile stress at any point in the inclusion reaches the critical value $\sigma_{cr}$, complete particle cracking or splitting is represented by a blunt elliptical crack. The orientation of the crack is normal to the maximum principal stress direction. In practice, more than one point may have exceeded the $\sigma_{cr}$ value at the end of each increment. A weighted averaging method is consequently implemented to determine a unique location of the crack. If the maximum principal stress distribution in the inclusion is $\sigma_{ij}(x, y)$, the location of the crack is given as

$$
x_{damage} = \frac{\sum x \sigma_{ij}(x, y) / \sigma_{cr}}{\sum \sigma_{ij}(x, y) / \sigma_{cr}} \forall [\sigma_{ij}(x, y) \geq \sigma_{cr}]
$$

$$
y_{damage} = \frac{\sum y \sigma_{ij}(x, y) / \sigma_{cr}}{\sum \sigma_{ij}(x, y) / \sigma_{cr}} \forall [\sigma_{ij}(x, y) \geq \sigma_{cr}]
$$

The orientation of the crack of the crack is perpendicular to the principle directions at $(x_{damage}, y_{damage})$ and its length determined from its orientation and shape of the particle.

While in many of the examples that are considered in the following chapters, the critical stress $\sigma_{cr}$ to failure is assumed to be a characteristic of the inclusion material, experimental evidence [48, 49, 50] suggests that particle fracture is strongly correlated to its size. SEM of damaged composites show that particles of larger sizes tend to fracture at lower macroscopic load levels than smaller particles. Curtin [86] and Amornskhai [87], among others, have developed a fracture mechanics based damage criterion that derive fracture strength of individual particles based on their size as well as their material properties. In such models, the particles are assumed to contain flaws. Critical stress to fracture in the particles are modeled based on
mode-I fast fracture of these flaws. In some of the examples considered in this thesis, one such fracture criterion has been employed. Consider the a particle of area $A$, whose characteristic length as per [53, 88, 89] is given by the circle of equivalent diameter $D = \sqrt{\frac{4A}{\pi}}$. The initial flaw size $c$ in the particle is assumed to be a fraction of its equivalent diameter through $c = eD$, where $e \sim 5 - 15\%$. From a simple fracture mechanics viewpoint [84], for mode-I fracture, the critical load to fracture $\sigma_{cr}$ is related to the critical stress intensity factor $K_{IC}$ through the relation:

$$\sigma_{cr} = \frac{K_{IC}}{\sqrt{\Pi c}}$$

In the above relationship $K_{IC}$ is a material constant. It is therefore evident that larger particles (with larger initial flaws) tend to fracture at smaller critical loads. This simple criterion which can account for the experimental evidence is used as the fracture criterion to evaluate the critical load to fracture $\sigma_{cr}$ in individual particles.

4.7 Conclusions

In this chapter, the VCFEM has been extended to model damage in random heterogeneous media. Modifications to the variational principle to account for the new phase introduced in the form of a cracked/split particle have been discussed. Enrichment of stress functions due to the presence of the new phase are shown to extend naturally from its shape. The resulting finite element formulations and various aspects involved in its numerical implementation are also presented. Crack initiation criterion and possible alternative methods for critical load calculations are also discussed. Numerical examples to validate the finite element scheme are presented in the next chapter.
CHAPTER 5

NUMERICAL VALIDATION OF VCFEM FOR DAMAGED HETEROGENEOUS MATERIALS

5.1 Introduction

In this chapter, the effectiveness of the VCFEM in analyzing deformations in damaged heterogeneous media is demonstrated. VCFEM is compared with traditional displacement based FEM as well as with published results in the literature. Damage in the form of particle cracking and particle splitting are considered.

5.2 Square Edge Packed RME with a Pre-Damaged Circular Inclusion

In this example, a square edge packed RME consisting of a pre-damaged circular inclusion in a non-linear matrix material is studied under plane strain conditions. Figure (5.1) shows the RME and its loading conditions. The inclusion has a volume fraction $V_f = 20\%$ and consists of an elliptical crack with an aspect ratio of $a/b = 10$.

Material properties of the constituents are as follows:

Al-3.5% Cu Matrix

Young’s Modulus $E = 72 \text{ GPa}$, Poisson’s Ratio $\nu = 0.32$
Figure 5.1: Schematic for the RME with a $V_f = 20\%$ predamaged circular inclusion

Figure 5.2: (a) VCFE and (b) ABAQUS meshes for RME with a $V_f = 20\%$ predamaged circular inclusion
Figure 5.3: Macroscopic response of RME with $V_f = 20\%$ predamaged circular inclusions

Post yield behavior (Power law hardening) $\sigma_m = \sigma_0 \left( \frac{\varepsilon_m}{\varepsilon_0} + 1 \right)^N$, where the initial flow stress $\sigma_0 = 175$ MPa, the strain hardening exponent $N = 0.2$, and $\varepsilon_0 = \sigma_0/E$ is the uniaxial strain at yield.

SiC Inclusions

Young’s Modulus $E = 450$ GPa, Poisson’s Ratio $\nu = 0.17$

The RME is loaded in uniaxial tension perpendicular to the crack surface to a macroscopic tensile strain of $\varepsilon_{yy} = 0.5\%$ with repeatability conditions enforced on the surface $x = L/2$. VCFEM is compared with the displacement based finite element package ABAQUS.

The VCFE mesh used to analyze the problem is shown in figure (5.2a). The element boundary is discretized through 8 nodes into linear line elements. The crack
Figure 5.4: Microscopic tensile stress distribution of RME with $V_f = 20\%$ predamaged circular inclusions along (a) $y/b=0$ (b) $y/b=0.1$ (c) $y/b=0.25$ (d) $y/b=0.5$
boundary is modeled through 8 nodes into quadratic line elements. The inclusion boundary consists of a total of 12 nodes. Of these, 8 nodes (marked with a "x") are used to generate quadratic line elements that provide the required curvature of the circular inclusion. 4 additional nodes (marked with a "*") are used to better represent the sharp gradients of the displacement field near the crack tip. The inclusion stress function is generated using 25 polynomial terms (6-th order polynomial stress function, i.e. $p + q = 2..6$) and 36 reciprocal terms based on the shape of the crack (3 reciprocal terms for each polynomial exponent from 2 to 4, i.e. $i = p + q..p + q + 2 \forall p + q \in [2,4]$). In addition to these terms, the matrix stress function has an additional 9 reciprocal terms based on the conformal function for the circular inclusion (3 reciprocal terms for the polynomial exponent 2, i.e. $i = p + q..p + q + 2 \forall p + q = 2$). The corresponding ABAQUS mesh shown in figure (5.2b) consists of 1465 8-noded quadratic elements discretized through 6431 nodes.

The resulting macroscopic tensile response of the RME, shown in figure (5.3), depicts a good match between VCFEM and traditional displacement based FEM. Variation in stress fields near the crack tip are shown in figure (5.4). The results depict a good match between VCFEM and traditional FEM. It is significant to note that most of the stress carrying capacity is carried by the stiffer inclusion at the matrix/inclusion interface near the crack tip. Severe reductions in the microscopic tensile stresses can be seen in matrix part of the interfaces. Such phenomenon, termed crack tip amplification, have been reported for bi-material interfaces by Sugimura et.al. [46].
5.3 Square Diagonal Packed RME with Pre-Damaged Square Inclusions

In this example, results obtained by VCFEM simulation are compared with those presented in Finot et al. [47] for studying the effect of partial cracking and splitting. The representative material element (RME) consists of two square shaped SiC inclusions in an Al-3.5%Cu matrix with a volume fraction $V_f = 20\%$. The inclusions are arranged in square diagonal pattern as shown in figure (5.5). Material properties are as follows:

**Al-3.5% Cu Matrix**

Young’s Modulus $E = 72$ GPa, Poisson’s Ratio $\nu = 0.32$

Post yield behavior (Power law hardening) 

$$\sigma_m = \sigma_0 (\epsilon_m^p / \epsilon_0 + 1)^N$$

where $\sigma_m$ is the effective stress, $\epsilon_m^p$ is the effective plastic strain, $\sigma_0$ the initial flow stress, and $\epsilon_0$ is the strain at yield (i.e. $\epsilon_0 = \frac{\sigma_0}{E}$).

$\sigma_0 = 175$ MPa, and $N = 0.2$.

**SiC Inclusions**

Young’s Modulus $E = 450$ GPa, Poisson’s Ratio $\nu = 0.2$

The RME’s with pre-existing cracks denoted by 0% damaged (both inclusions intact), 50% damaged (one cracked inclusion) and 100% damaged (two cracked inclusions) are loaded in the vertical direction as shown in figure (5.5). Inclusion cracks in the VCFEM analysis are manifested by ellipses with an aspect ratio $a/b = 10$. The distinction between completely cracked inclusions and split inclusions is made by a parameter $d = \frac{\text{Crack Length}}{\text{Inclusion Dimension}}$. A fully cracked inclusion corresponds to a value $d = 1$, in which the crack terminates at the inclusion/matrix interface, whereas
splitting into two halves is represented by \( d = 1.004 \), for which crack tip has moved slightly into the matrix. The VCFE meshes used in this example for the 3 RMEs is shown in figure (5.6). With the addition of a crack in the particle, two essential features are incorporated into the discretization of the RME. The blunt crack in the particle is represented as an elliptical boundary with an aspect ratio of \( a/b = 10 \).

An additional node (marked as a \(*\) in figures 5.6a, b and c) is also introduced on the boundary of the inclusions. These nodes are used to better represent the displacement field of the inclusion boundary near the crack tip. As has been deduced in Example 2 of Chapter 3, for undamaged elements the stress field in the matrix is represented by a 61 term expansion and the stress field in the inclusion is represented by a 25 term expansion. At the onset of damage, the matrix and the inclusion stress fields have an additional 36 terms based on conformal mapping of the elliptical crack \((i = p + q..p + q + 2 \forall p + q = 2..4)\) as has been discussed in equation (4.5).

Macroscopic or overall stress-strain response is computed by taking volumetric averages of respective microscopic variables, and are compared with those of [47] in figure (5.7). For fully cracked inclusions \((a = 1)\), the response of 0% and 50% damaged RME’s are in excellent agreement with those in [47]. For the 100% damaged RME, good agreement is achieved up to a macroscopic strain of \( \varepsilon_{yy} = 0.5\% \), beyond which the VCFEM results depict a slightly larger macroscopic stress. The stiff response may be attributed to the fact that VCFEM analysis has been conducted with a small deformation kinematic assumption. At larger macroscopic strains, regions near the crack tip undergo large plastic deformations and consequently rotation of material elements should be considered for more accuracy. This is evident from contour plots of the effective plastic strains at a macroscopic tensile strain \( \varepsilon_{yy} = 2\% \).
Figure 5.5: Schematic for the RME with $V_f = 20\%$ predamaged square shaped inclusions (a) 0\% damage (b) 50\% damage (c) 100\% damage

Figure 5.6: VCFEM meshes for RME with $V_f = 20\%$ predamaged square shaped inclusions (a) 0\% damage (b) 50\% damage (c) 100\% damage
Figure 5.7: Macroscopic tensile response of RMEs with predamaged square shaped inclusions

shown in figure (5.8). For the 0% damaged RME (not shown) the maximum effective plastic strain is 11%, while those for the 50% and 100% damaged RME’s are 39% and 64% respectively. A small deformation analysis of the 100% damaged RME is also carried out using ABAQUS. Fig. (5.9a) depicts the mesh used in the analysis. The ABAQUS mesh consists of 12740 nodes which discretize the RME into 4193 QUAD8 quadratic elements. The mesh was chosen after a few trial runs, in which the element size was gradually reduced so as to obtain a sufficiently converged distribution of effective plastic strains in most regions of the RME. The resulting effective plastic strain distribution at $\bar{\varepsilon}_{yy} = 2\%$ is shown in figure (5.9b). Comparison of this distribution with the corresponding distribution generated by VCFEM (in figure 5.8c) ascertains the accuracy of the VCFEM. Both distributions show similar cutoff values throughout the RME with minor discrepancies in the extent of the contour lines.
Figure 5.8: Effective plastic strain (%) distribution for pre-damaged RMEs with particle cracks at a macroscopic tensile strain of $\varepsilon_{yy} = 2\%$; (a) 50% Damage (b) 100% Damage

Figure 5.9: (a) Conventional finite element mesh (b) distribution of effective plastic strain (%) at $\varepsilon_{yy} = 2\%$ for 100% predamaged RME with square shaped inclusions with particle cracking generated by ABAQUS.
Figure 5.10: Distribution of effective plastic strain (%) at $\varepsilon_{yy} = 2\%$ near the crack-tip for 100% predamaged RME with square shaped inclusions with particle cracking generated by (a) VCFEM and (b) ABAQUS.

Figure 5.11: Effective plastic strain (%) distribution for pre-damaged RMEs with particle splitting at a macroscopic tensile strain of $\varepsilon_{yy} = 2\%$; (a) 50% Damage (b) 100% Damage
However at the crack tip, the VCFEM shows a larger plastic strain than ABAQUS. Contour plots of the plastic strain distribution generated by VCFEM and ABAQUS for a window of size $b \times b$ at the crack tip is shown in figure (5.10). Even though the distribution of the contour lines are similar, the ABAQUS results indicate a larger extent of plastic straining than VCFEM. Coarser ABAQUS meshes with 11043 nodes and 8169 nodes generated respectively an equivalent plastic strain of 37% and 51% at the crack tip. The discrepancy between ABAQUS and VCFEM results at the crack tip indicates that although the ABAQUS mesh has been discretized in great detail throughout the RME, regions near the crack tip might need further refinement to produce a rapidly fluctuating stress field generated by VCFEM. The dimensions of the window under consideration is very small when compared to the dimensions of the RME ($b \approx \frac{L}{50}$) and therefore such an analysis has not been carried out in this work.

For the case of particle splitting ($d = 1.004$) the response of both 50% and 100% damaged RME's are in excellent agreement with those in [47]. It is noted that the stress carrying capacity of the material element reduces considerably with the transition from full particle cracking to particle splitting. As the crack grows beyond the interface, there is no load transfer between the two halves of the inclusions and consequently the entire load has to be carried by the matrix material and the remainder of undamaged particles. Contour plots of the effective plastic strains at $\varepsilon_{yy} = 2\%$ in figure (5.11), show that portions above the split particles have drastically reduced plastic strains, since they no longer carry any of the load. It is also important to note that in the case of particle splitting, a considerably larger plastic strain accumulates near the crack tip. Also plastic strains tend to flow in the form of ligaments from one
crack tip to the next, causing bands of strain localization. Similar observations have been made by Finot et. al.[47] with axisymmetric particles.

5.4 **Effect of Damage Level on the Stress Carrying Capacity of RMEs**

In this example, the effect of selectively damaged particles on the overall material response is analyzed and compared with predictions made in Bao[44] and Brockenbrough & Zok[90]. Analysis in [44] and [90] are axisymmetric, implying three dimensional unit cells with spherical inclusions and penny shaped cracks. Complete particle splitting is considered in this example, i.e. \( a = 1.004 \). Figure (5.12) shows damaged brittle inclusions in a surrounding of undamaged matrix and inclusions, with loading in a direction perpendicular to the crack length. A parameter \( \rho \) is used as an indicator of the extent of damage. In the VCFEM analysis, five values of \( \rho = 0, 0.25, 0.33, 0.375 \) and 1 are considered.

Material properties used are:

**Ductile Matrix**

Young's Modulus \( E = 70 \) GPa, Poisson's Ratio \( \nu = 0.33 \)

Post yield behavior (Ramberg-Osgood Law) \( \varepsilon_p^m / \varepsilon_0 = \alpha (\sigma_m / \sigma_0)^n \)

where \( \sigma_m \) is the effective stress, \( \varepsilon_p^m \) is the effective plastic strain, \( \sigma_0 \) the initial flow stress, \( \varepsilon_0 \) is the strain at yield \( (\varepsilon_0 = \sigma_0 / E) \), and \( n \) and \( \alpha \) are material parameters.

\( \sigma_0 = 43 \) MPa, \( n = 10 \), and \( \alpha = \frac{3}{7} \).

**Brittle Inclusions**

Young's Modulus \( E = 350 \) GPa, Poisson's Ratio \( \nu = 0.2 \)

The matrix material in [44] is characterized as rigid-plastic, while [90] employs the
Figure 5.12: Schematic representation of partially damaged RMEs (a) $\rho = 0$, (b) $\rho = 0.25$, (c) $\rho = 0.33$, and (d) $\rho = 1$
Figure 5.13: Macroscopic tensile stress response of partially damaged RMEs as a function of (a) Damage parameter $\rho$, and (b) Volume fraction $\phi$. 
Ramberg-Osgood law in their analysis. For undamaged VC elements, the stress field in the matrix is represented by a 34 term expansion generated using 25 polynomial terms (6th order complete polynomial expansion of the Airy function, i.e. \( p+q = 2..6 \)) and and 9 reciprocal terms (3 reciprocal terms for each polynomial exponent of 2, i.e. \( i = p + q..p + q + 2 \forall p + q = 2 \)), while the stress field in the inclusions are modeled using only the 25 polynomial terms. Fewer reciprocal terms are used than in the previous example due to the smooth interface for circular inclusions. For damaged elements though, the additional reciprocal terms are the same as in the previous example (\( i = p + q..p + q + 2 \forall p + q = 2..4 \)).

The stress capacity as a function of the damage parameter \( \rho \) for various volume fractions are shown in figure (5.13a), in which \( \sigma/\sigma_m \) represent the ratio of the macroscopic stress of the RME to that in the matrix material at identical macroscopic strain levels. This is a measure of the strengthening or weakening of the composite due to the presence of partially damaged stiffer inclusions. As in [44] and [90], these plots are for a macroscopic strain level of \( \epsilon_{yy} = 10\epsilon_0 \). The results indicate a near linear variation of the stress with \( \rho \) at all volume fractions, as concluded in [44] and [90]. Weakening of the fully damaged RME's (\( \rho = 1 \)) is more drastic with increase in the inclusion volume fraction, since less matrix material is available to carry the load. Plots of the macroscopic stress as a function of the inclusion volume fractions, at various damage levels is depicted in figure (5.13b). Except for the fully damaged case (\( \rho = 1.0 \)), the surrounding undamaged inclusions lead to a stiffer response of the composite with increasing volume fraction, compared to the matrix material (\( V_I = 0\% \)). However when all particles are damaged, i.e. \( \rho = 1.0 \), the load carrying capacity of the RME
reduces significantly with increasing volume fraction. Good qualitative agreement is obtained with [44, 90] for $\rho = 0, 1$, even though both these papers consider axisymmetric unit cells.

5.5 Evolving Damage in a Square Edge Packed RME with a Circular Inclusion

In all the examples considered so far in this chapter, the material predamaged with cracked/split particles. However, as has been discussed in section 4.6, in actual materials particle fracture occurs due to applied loading of the microstructure. The influence of intermediate particle cracking/splitting on the macroscopic and microscopic response of the material is examined in this example. The RME consisting of a $V_f = 5\%$ initially undamaged circular inclusion is shown in figure (5.14). The
material properties of the constituents are as follows

**Al-3.5% Cu Matrix**

Young’s Modulus $E = 72$ GPa, Poisson’s Ratio $\nu = 0.32$

Post yield behavior (Power law hardening) $\sigma_m = \sigma_0(\epsilon_m^p/\epsilon_0 + 1)^N$

where $\sigma_m$ is the effective stress, $\epsilon_m^p$ is the effective plastic strain, $\sigma_0$ the initial flow stress, and $\epsilon_0$ is the strain at yield (i.e. $\epsilon_0 = \frac{\sigma_0}{E}$).

$\sigma_0 = 175$ MPa, and $N = 0.2$.

**SiC Inclusions**

Young’s Modulus $E = 450$ GPa, Poisson’s Ratio $\nu = 0.2$

The critical load to fracture of the SiC inclusions are taken to be $\sigma_{cr} = 275$MPa. The RME is loaded to a maximum macroscopic tensile strain of $\epsilon_{yy} = 2\%$ and analyzed
under plane stress conditions. The stress functions for the two phases of the undamaged RME are the same as those used in section 3.2, while those for the damaged RME are the same as the ones used in section 5.2. As in the last two examples in this chapter, for the particle cracking case the ratio \( d = \frac{\text{Crack Dimension}}{\text{Inclusion Dimension}} \frac{a}{R} = 1.0 \) and for the particle splitting case the ratio \( d = 1.004 \).

The resulting macroscopic response over the entire loading process is shown in figure (5.15). The inclusion cracked at a macroscopic tensile strain of \( \bar{\varepsilon}_{yy} = 0.2\% \) as indicated by the sudden drop in the macroscopic response of the RME. This drop is associated with the redistribution of microscopic stresses due to fracture of the
Figure 5.17: Redistribution of microscopic stress (in GPa) for RME with $V_f = 5\%$ initially undamaged circular inclusion at $\varepsilon_{yy} = 0.2\%$ (a) just before particle splitting (b) just after particle splitting.

The drop in load carrying capacity is slightly lower for the particle splitting case. For the particle cracking case, post-damage response of the composite is slightly below that of the undamaged composite but remains well above that of the matrix material at all stages of the loading. On the other hand, for the particle splitting case, the post-damage response stays well below that of the matrix material at all stages of the loading. These results are consistent with observations made in sections 5.3 and 5.4 for a damage parameter $\rho = 1$. The evolution of stresses with fracture for the particle cracking/splitting are shown respectively in figures (5.16 and 5.17). These plots are made at the same macroscopic strain level $\varepsilon_{yy} = 0.2\%$. For both particle cracking and splitting, it can be seen that the microscopic stresses instantaneously redistribute to the crack tips.
Figure 5.18: Effective plastic strain (%) for RME with $V_f = 5\%$ initially undamaged circular inclusion with intermediate particle cracking at (a) $\bar{\varepsilon}_{yy} = 0.2\%$ (b) $\bar{\varepsilon}_{yy} = 0.4\%$ (c) $\bar{\varepsilon}_{yy} = 1.0\%$ and (d) $\bar{\varepsilon}_{yy} = 2.0\%$
Figure 5.19: Effective plastic strain (%) for RME with $V_f = 5\%$ initially undamaged circular inclusion with intermediate particle splitting at (a) $\varepsilon_{yy} = 0.2\%$ (b) $\varepsilon_{yy} = 0.4\%$ (c) $\varepsilon_{yy} = 1.0\%$ and (d) $\varepsilon_{yy} = 2.0\%$
with the maximum stress concentrated at the particle side of the matrix/inclusion interface. It can also be seen that the maximum stress concentration is higher for the particle splitting case. The evolution of plastic strains with continued loading for the particle cracking/splitting cases are shown respectively in figures (5.18 and 5.19). These plots show that for both particle cracking/splitting case, the plastic strains begin to grow around the crack tip. The maximum value of plastic strain before fracture in both cases was \( \varepsilon_{m}^{p}\mid_{\text{max}} = 0.59\% \) and is along the interface at an angle of 45° from the loading direction. For the particle cracking case (see figure 5.18b), this value increases to \( \varepsilon_{m}^{p}\mid_{\text{max}} = 22.57\% \) at the next macroscopic strain level of \( \varepsilon_{yy} = 0.4\% \) with the maximum value recorded at the crack tip. With continued loading, the plastic strains continue to increase at the crack tip. However other regions along the interface continue to be support some of the macroscopic load as is evident from the continued straining of these regions in figures (5.18c and d). Consequently, growth of plastic strains ahead of the crack tip is less severe. As can be seen from figure (5.19b), for the particle splitting case, the maximum plastic strain is \( \varepsilon_{m}^{p}\mid_{\text{max}} = 54.21\% \) at the first post-damage step corresponding to a macroscopic tensile strain of \( \varepsilon_{yy} = 0.4\% \). Even at this macroscopic strain level, it is evident that plastic straining is concentrated ahead of the crack tip. Figures (5.19 c and d) show that with continued macroscopic loading plastic strains tends to localize ahead of the crack tip. No growth in plastic strains is visible for other regions along the matrix/inclusion interface. As has been noted in section5.3, these observations are attributable to the fact that split particles completely damage the inclusion, causing the macroscopic loads to be transferred to regions of the RME that are away from the particle/matrix interface. Larger plastic strains contours ahead of the crack tip for the particle splitting case also indicate that
matrix damage will most likely occur in these regions and will ultimately evolve into catastrophic failure of the material.

5.6 Conclusions

Numerical examples to validate VCFEM for damage in heterogeneous microstructures have been discussed in this chapter. Comparisons with traditional FEM and with published results establish the accuracy of VCFEM in modeling complex deformations in damaging materials. Crack enriched stress functions introduced into the two phases of the damaged BSE provide an effective representation of the microscopic stress fields in these phases. Examples with inclusions of varied shapes and damage levels indicate the applicability of VCFEM for random media. VCFEM is also shown to be able to account for evolving damage in the microstructure. Effect of particle cracking and splitting on the evolution of macroscopic/microscopic variables provide important insights into the actual deformation processes in damaged heterogeneous media. In the next chapter several examples illustrating damage modeling capabilities of VCFEM for complex microstructures is presented.
CHAPTER 6

VCFEM FOR DAMAGE IN RANDOM HETEROGENEOUS MEDIA

6.1 Introduction

Analysis of damage in simple microstructures, like the ones presented in the previous chapters, provide valuable information on evolving failure mechanisms in heterogeneous materials. However, analysis of actual mesostructures [48, 49, 50, 22, 54, 51, 52] reveal morphological characteristics also play a significant role in the failure mechanisms of such materials. Particle size, shape and proximity can adversely effect damage initiation and its subsequent evolution in the microstructure. Some of these effects, for random microstructures, is presented in this chapter. Particle clustering and shape effects are examined through VCFE analysis of computer simulated microstructures. A comparison of VCFEM with experimental results for actual microstructures is also presented. Damage in the microstructure is modeled as particle cracking/splitting, with its initiation triggered as a material and geometric property. Consequent straining of the matrix and its implications towards macro damage are discussed.

Significant efforts to link stereological features like spatial distribution, size, shape and local volume fraction with overall properties of random microstructures have
been made by Hunt et.al.[49, 48], Pryz[91, 92] and Ghosh et.al.[88, 89]. In [48, 49] Al-Si composite systems, similar to the ones used in this chapter, were tessellated for characterization and modeled by conventional finite element methods. Analytical expressions for stress fields have been derived in [91, 92] for utilization in an unique marked correlation function, which depict the effect of material morphology on the evolution of stress/deformation field of its constituents. Ghosh et.al[88, 89] have integrated the two approaches with VCFEM to study the effect of a vast array of complex geometric patterns on the response of undamaged heterogeneous media. In this chapter, some of these ideas are extended to damaged random media and there effectiveness in representing failure in actual materials discussed.

6.2 Damage in Computer Simulated Complex Microstructures

6.2.1 Clustering effects on damage evolution

The effect of particle clustering on damage evolution is studied with three computer generated microstructural distributions. The representative material elements (RME) are classified as follows, and are shown in figure (6.1).

(a) A hard core distribution: which is generated as a variant of a pure random Poisson pattern through the imposition of two constraints, namely (a) no two inclusions are allowed to overlap, and (b) all inclusions are completely contained within the region being analyzed.

(b) A single cluster hard core distribution which is characterized by a decreased average inclusion minimum permissible distance within a subregion of an otherwise hardcore distribution.
(c) *Triple cluster hard core model*, which is generated in the same way as the single cluster model with three pre-determined cluster locations.

Details of the generation process are presented in [88]. Each RME consists of 50 equi-sized circular Si particles, constituting a 20% volume fraction, dispersed in an Al-Si-Mg alloy matrix. The size of the RME is taken to be 1x1 and the diameter of each particle is 0.0742. The cluster diameters for the single and triple clusters are set at 0.1669 and 0.1289 respectively. Material properties for the constituents of this composite are given in from Hunt[49]. All particles are of identical shape and size in this problem, and consequently the critical stress to failure is assumed to be a constant for all particles in the analysis. This is a problem of evolving microstructural damage, and hence two values of critical failure stresses, viz. $\sigma_{cr} = 300$ MPa and $\sigma_{cr} = 500$ MPa, are examined. The RME’s with initially undamaged Si particles are loaded in
Figure 6.2: (a) Cumulative distribution function and (b) Probability density function of local area fractions for 20% circular Si particles in Al-Si-Mg Matrix

uniaxial tension in the horizontal direction to a macroscopic tensile strain $\varepsilon_{xx} = 2\%$. The stress functions for the Al-Mg matrix and Si inclusions of undamaged/damaged voronoi cells are the same as those used for circular inclusions in the previous chapter. Both complete particle cracking and particle splitting are studied in this example.

To characterize the spatial distributions, statistical functions of some geometric descriptors are considered to discriminate between the patterns. Details of these functions have been discussed in [88, 89]. Figures (6.2a and b) show the cumulative distribution function $F(A)$ and the probability density function $f(A)$ of the local area fraction for the three patterns. The local area fraction is measured as a ratio of the particle size to the area of the associated Voronoi cell. As the area fraction increases, $F(A)$ shows significant differences between the hard core and the clustered patterns.
Figure 6.3: (a) Cumulative distribution function and (b) probability density function of nearest neighbor distance for 20% circular Si particles in Al-Si-Mg matrix

Figure 6.4: (a) Second order intensity function and (b) Pair distribution function for 20% circular Si particles in Al-Si-Mg Matrix
due to wider dispersion. The high spike in the density distribution function $f(A)$ for the hardcore pattern is a consequence of the steep gradients due to pronounced uniformity in local area fraction. Intensity of spikes in $f(A)$ diminishes with clustering, reflecting lower gradients in $F(A)$. The cumulative distribution function $F(d)$ and density distribution functions $f(d)$ for center to nearest neighbor distances are plotted in figures (6.3a and b). Plateaus in $F(d)$, and consequently the zero values in $f(d)$ correspond to relatively large distances for which a near neighbor does not exist. Spikes in $f(d)$ correspond to the number of neighbors at nearly similar distances, and the wide plateaus correspond to uniformly increasing distances. $F(d)$ and $f(d)$ for the hardcore pattern have prolonged tails due to large near-neighbor distances. The difference in lowest values of $d$ is however reduced and relatively narrower plateaus occur at shorter distances in clustered patterns.

Second order intensity function $K(r)$ is also an informative descriptor of spatial dispersions because of its sensitivity to local perturbations in otherwise similar distributions (see Pryz\[91, 92\]. It is defined as the number of additional points or particle centers expected to lie within a distance $r$ of an arbitrarily located point, divided by the point density. For observations within the finite RME size, edge effects should be incorporated in $K(r)$ and the corresponding expression is given in [91, 88]). Furthermore, its derivative the pair distribution function $g(r) = \frac{1}{2\pi r} \frac{dK(r)}{dr}$, corresponds to the probability $g(r)d(r)$ of finding an additional point within a circle of radius $dr$ and centered at a particle. The two functions are plotted for the three patterns in figure (6.4a and b) and compared with a pure Poisson process for which $K(r) = \pi r^2$ and $g(r) = 1$. With the increase in clustering $K(r)$ deviates from that for the Poisson
process, indicating a greater likelihood of encountering additional particles at lower sampling radii. The peaks in $g(r)$ correspond to the most frequent distances, and are more pronounced for the hardcore distribution at this volume fraction. Cumulative distribution functions and second order intensity functions provide an efficient description of the clustering in the material morphology and their implications towards damage will also be discussed later in this example.

Stress functions chosen in the example are the same as those in section 5.4. Both complete particle cracking and particle splitting are analyzed. The macroscopic response for the particle cracking case at a critical stress of $\sigma_{cr} = 300\text{MPa}$ is shown in figure (6.5) where drops in load carrying capacity is associated with particle cracking. Evolving damage configurations and the resulting distribution of effective plastic
Figure 6.6: Damage configurations for hard core pattern with particle cracking and $\sigma_{cr} = 300$MPa at (a) $\varepsilon_{xx} = 0.8\%$, (b) $\varepsilon_{xx} = 1.4\%$ and (c) $\varepsilon_{xx} = 2.0\%$

Figure 6.7: Effective plastic strain (%) for hard core pattern with particle cracking and $\sigma_{cr} = 300$MPa at (a) $\varepsilon_{xx} = 1.4\%$ and (b) $\varepsilon_{xx} = 2.0\%$. 

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Figure 6.8: Damage configurations for triple cluster pattern with particle cracking and $\sigma_{cr} = 300$MPa at (a) $\varepsilon_{xx} = 0.6\%$, (b) $\varepsilon_{xx} = 1.4\%$ and (c) $\varepsilon_{xx} = 2.0\%$

Figure 6.9: Effective plastic strain (%) for triple cluster pattern with particle cracking and $\sigma_{cr} = 300$MPa at (a) $\varepsilon_{xx} = 1.4\%$ and (b) $\varepsilon_{xx} = 2.0\%$. 

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strain for hard core pattern are shown respectively in figure (6.6) and figure (6.7). The first set of particles crack at a macroscopic strain of $\varepsilon_{xx} = 0.6\%$. However due to the lack of close proximity of cracked particles in this pattern, damage in the microstructure does not propagate in any preferential direction. Particle cracking occurs at random locations with increased loading up to an overall strain of $\varepsilon_{xx} = 1.6\%$, after which no additional cracking is noticed. The plastic strain distribution indicates large strains near the crack tip of the damaged particles with no preferred direction of plastic straining into the matrix. Corresponding damage configurations and distribution of effective plastic strain for the triple cluster pattern are shown respectively in figure (6.8) and figure (6.9). The first set of particles (the cluster in the top-right corner) cracked at a macroscopic tensile strain of $\varepsilon_{xx} = 0.4\%$. With further loading, particles in this cluster cracked. Continued damage in the top-right cluster propagates to the nearby cluster (the cluster in the bottom-center as shown in figure 6.8), while particles in the third cluster remained relatively undamaged. At the end of the macroscopic loading, particles in the first two clusters were almost completely damaged, while the third cluster was still carrying some of the load. It is also interesting to note that even though the cluster in the top-right corner was the first damaged, a continuously high strain contour can be seen in cluster in the bottom-center of the RME (see figures 6.9a and b). Proximity of the crack tips for the bottom-center cluster have facilitated plastic flows in this region. The final plastic strain distribution in figure (6.9b) clearly indicates that a matrix-crack will most likely develop at the bottom center cluster, and probably travel towards the top-right cluster to form a of macro-crack in the material.
Figure 6.10: Damage configurations for triple cluster pattern with particle splitting and $\sigma_{cr} = 300$MPa at (a) $\bar{e}_{xx} = 0.8\%$, (b) $\bar{e}_{xx} = 1.4\%$ and (c) $\bar{e}_{xx} = 2.0\%$

Figure 6.11: Effective plastic strain (%) for triple cluster pattern with particle splitting and $\sigma_{cr} = 300$MPa at (a) $\bar{e}_{xx} = 1.4\%$ and (b) $\bar{e}_{xx} = 2.0\%$. 
Figure 6.12: Damage configurations for triple cluster pattern with particle splitting and \( \sigma_{cr} = 500\text{MPa} \) at (a) \( \varepsilon_{xx} = 0.8\% \), (b) \( \varepsilon_{xx} = 1.4\% \) and (c) \( \varepsilon_{xx} = 2.0\% \).

Figure 6.13: Effective plastic strain (\%) for triple cluster pattern with particle splitting and \( \sigma_{cr} = 500\text{MPa} \) at (a) \( \varepsilon_{xx} = 1.4\% \) and (b) \( \varepsilon_{xx} = 2.0\% \).
Figure 6.14: Macroscopic stress-strain response for computer generated microstructures due to particle cracking and splitting
In order to study progression of damage in the microstructure, the analysis is carried out assuming particles split completely to form matrix cracks. Two critical stresses to failure of $\sigma_{cr} = 300\text{MPa}$ and $\sigma_{cr} = 500\text{MPa}$ are examined in the analysis. The evolving damage configurations of the triple cluster pattern for the particle splitting case are shown in figures (6.10 and 6.12). At a critical stress of $\sigma_{cr} = 300\text{MPa}$, particles in the top right cluster begin to crack at a macroscopic strain level of $\varepsilon_{xx} = 0.4\%$. In contrast to the particle cracking case, with continued loading, particles in this cluster are damaged and simultaneously particles in the bottom-center cluster are also damaged (for eg. at a strain level of $\varepsilon_{xx} = 1.2\%$). Such a phenomenon indicates a much faster rate of damage evolution for the particle splitting case. At the final macroscopic tensile strain of $\varepsilon_{xx} = 2.0\%$, particles in the top-right and bottom-center cluster are damaged, while damage is being initiated for particles in the top-left cluster. Plastic strain contours indicate considerable plastic straining in the top-right and bottom-center clusters. When compared to the plastic strain distributions for the particle cracking case in figure (6.9), two essential features can be observed. Firstly, high strain contour lines are much thinner for the matrix cracking case. Secondly, for the matrix cracking case, the high strain contour lines form a larger continuous damage region in the matrix of the RME. These observations are similar to the ones made in example 3.1. Thinness in high strain contour lines are associated with smaller regions in the matrix (i.e. primarily between crack tips) that are available for plastic straining. A more continuous damage region is associated with a much lower load carrying capacity of RMEs with matrix cracks. At a critical stress of $\sigma_{cr} = 500\text{MPa}$, particles in the top right cluster begin to crack at a higher macroscopic strain level of $\varepsilon_{xx} = 1.0\%$. Continued loading of the RME,
results in further splitting of particles in this cluster. At the final macroscopic strain of $\varepsilon_{xx} = 2.0\%$ most of the particles in the top-right cluster are damaged but only one particle in the bottom-center cluster is damaged. Consequently, the effective plastic strain distribution for a critical stress of $\sigma_{cr} = 500\text{MPa}$ shown in figure (6.13), show matrix failure is limited to the top-right cluster. The macroscopic stress-strain responses of the hard core and triple cluster RMEs are illustrated in figure (6.14), where abrupt drops due to particle cracking are smoothened. The hard core pattern generally shows continuous drop in the stress level throughout the loading. For the clustered microstructure, drops are higher in the initial stages due to rapid failure in the clusters, followed by increase in the stress levels due to matrix hardening. In general the RME with cracked particles projects a considerably stiffer behavior when compared to that with split particles. This observation is also made for simple microstructures.

An important criterion in determining length scales that characterize a RME, is the influence of local morphology on microscopic stress/strain distributions. Sensitivity of stress/strain distributions to local perturbations in the morphology can provide important insights into the effect of variations in microstructural patterns on the deformation in the microstructure. This can in turn be used to predict required dimensions of the RME, beyond which the morphology does not significantly influence the microstructural deformations. Pryz [92] has introduced a “marked correlation function” for multivariate characterization of geometric patterns. By associating with each particle a field variable or a mark (say the principal stress in the inclusion to represent level of damage) and comparing the marks of nearby particles with the
Figure 6.15: Mark correlation function of computer generated microstructures with particle splitting and $\sigma_{cr} = 300$MPa for (a) ratio of maximum principal stress to critical failure stress ($\sigma_{cr}$) (b) average effective plastic strain in each Voronoi cells

distribution function that characterizes the geometric pattern (say the second order intensity function $K(r)$ to represent clustering), the marked correlation function establishes the effect of microstructural morphology on the compared field variable. Mathematically, the marked correlation function $M(r)$ for a heterogeneous domain $A$ containing $N$ particles is expressed as:

$$M(r) = \frac{dH(r)}{g(r)}$$

where

$$H(r) = \frac{1}{m^2} \sum_{i=1}^{N} \sum_{k=1}^{k^i} m_i m_k(r)$$  \hspace{1cm} (6.1)

Here $m_i$ denotes the mark associated with the i-th particle, $k^i$ is the number of particles centers within a circle of radius $r$ centered at the i-th particle, and $m$ is the mean of all marks. $H(r)$ is termed the mark intensity function and its derivative $\frac{dH(r)}{dr}$ can be thought of as the density distribution of the marks in the heterogeneous domain. Thus, the ratio of mark density $\frac{dH(r)}{dr}$ with pair distribution function $g(r) = \frac{dK(r)}{dr}$.
provides a measure for the effect of local morphology on the representative field variable.

Two marks that are relevant to damage evolution are considered in this example. They are:

(a) A parameter $R_{ps}$ signifying the propensity of a particle, in relation to others, to advance the damage state of the microstructure. For an undamaged particle $R_{ps}$ is quantified as the ratio of the maximum principal stress to the critical failure stress $\sigma_{cr}$. For a damaged particle, for which $\frac{\sigma}{\sigma_{cr}}$ is 1, $R_{ps}$ is taken to be the ratio of the current overall strain to the strain at which the particle had cracked.

(b) the average effective plastic strain $\bar{\varepsilon}^p$ in each Voronoi cell, which is used to characterize evolving matrix failure due to presence of damaged particles.

$M(r)$ for the three patterns are compared that for an uniform microstructure which is unity. For the hard core pattern the functions rapidly approach unity, while those for the clustered patterns are significantly slower. Higher $M(r)$ for the clustered patterns at short range sampling distances $r$ represent significantly larger influence of the damage marks at these distances. Furthermore, $M(r)$ for $\bar{\varepsilon}^p$ has a higher correlation at short sampling distances, indicating severe matrix straining near damaged particles. The slower attenuation of $M(r)$ for $R_{ps}$ at short-medium range indicates that particle cracking is the primary mode of damage evolution. Experimental observations by Davidson [51], Majumdar [52] as well as with computational results by Finot et.al. [47] however suggest matrix cracking a a major contributor the the microstructural damage evolution process for MMCs. The faster decay of average plastic strain points to the necessity of incorporating matrix damage in the VCFE
Figure 6.16: Voronoi cell meshes for $V_f = 20\%$ elliptical Si particles in Al-Si-Mg matrix of (a) Fixed size and horizontal Orientation (EH) (b) Fixed size and random orientation (ER) (c) Random size and random orientation (RR)

model, which is currently under investigation. The mark correlation function is an effective tool to understand the sensitivity of damage variables to local perturbations in the morphology, and can provide a criterion for determining the optimal RME size.

6.2.2 Shape and orientation effects on damage evolution

In the next example, the effect of shape and orientation of particles on damage evolution is studied through 3 computer simulated 1x1 RMEs consisting of elliptical Si particles in an Al-Mg matrix. The distribution of particles along with the tessellated voronoi cell meshes are shown in figures (6.16 a b and c). Microstructures considered consist of particles of (a) fixed size and horizontal orientation ($EH$) (b) fixed size and
Figure 6.17: (a) Cumulative distribution function and (b) Probability density function of particle orientation for 20% Al-Si-Mg composite $ER$

Figure 6.18: (a) Cumulative distribution function and (b) probability density function of form factors for 20% Al-Si-Mg composite $RR$
random orientation (ER) and (c) random size and random orientation (RR). The
hardcore distribution used in the previous examples is used as a base for generating
the particle centers of all 3 RMEs. Consequently, the second order intensity function
$K(r)$ and pair distribution function $g(r)$ for all the distributions in this example are
the same as those for the hardcore distribution shown in figure (6.4). Distribution
of particle orientation is measured through the angle made by the major axis of the
particles with the horizontal axis ($0^\circ \leq \text{Orientation} < 180^\circ$). Cumulative distribution
and probability density function for the orientations of particles in RME ER is shown
in figure (6.17). They indicate a fairly uniform distribution at most orientations, with
the exception of the $0^\circ$ orientation. Distribution of heterogeneity shapes is quantified
through a form factor $F \leq 1$ suggested in [48, 49, 88]. Formally, the form factor is
defined as the square of the ratio between perimeters of the equivalent circle to that
of the particle. For elliptical inclusions with major/minor axis dimensions $a/b$ it is
expressed as [88]:

$$F = \frac{4\pi R^2}{\text{perimeter}^2} R = \sqrt{ab} \quad \text{perimeter} \approx \pi [1.5(a + b) - \sqrt{ab}]$$

The dimensionless form factor $F$ is unity for uniform circular heterogeneities, and
decreases with increasing irregularity in shape. Cumulative distribution and proba-
bility density functions for the form factors of Si particles in RME RR, shown in
figure (6.18), indicate a fairly uniform distribution in shapes for particles in the RME
with $0.75 < F < 1$. The material properties as well as the stress functions of the con-
stituents are the same as in the previous example, with damage in the heterogeneities
initiated at $\sigma_{cr} = 300\text{MPa}$ and modeled as particle splitting. The RMEs are loaded in
uniaxial tension to macroscopic tensile strain of $\varepsilon_{xx} = 2\%$ and analyzed under plain
strain conditions.

The macroscopic response of the three RMEs is shown in figure (6.19). Evolution of damage, in the form of split particles for RMEs EH, ER and RR are shown respectively in figures (6.20, 6.21 and 6.22). At the initial stages of the loading, Si particles in RME ER undergo the lesser amount of damage than those in RME EH. Consequently RME ER exhibits the stiffer response than RME EH. However with increased loading, more particles in RME ER begin to fail and its load carrying capacity drops below that of RME EH. Load carrying capacity of RME RR, on the other hand, remains well below the other two microstructures at all phases of the deformation. It is interesting to note that, even though the damage level of both RME ER and RME RR remain below that of RME EH throughout the deformation, their load carrying capacity drops below that of RME EH at least towards the later stages of deformation. Randomness in orientation and shape of the particles in RMEs ER and RR has resulted in a greater part of the cross-sectional area being occupied by damaged particles. Consequently, with progressive damage, lesser amounts of the matrix material are available in the 2 RMEs to withstand the applied load. Such a phenomenon in turn leads to increased straining of the matrix material as can be seen from figures (6.23, 6.24 and 6.25). For RME EH, the plastic strain distribution remains concentrated at the crack tip of damaged inclusions, with the remainder of the matrix material continuing to carry the applied load as can be seen in figure (6.23). For RME ER, the plastic strain distribution shown in figure (6.24) is concentrated over certain regions of the RME, with the remaining matrix material
Figure 6.19: Macroscopic stress-strain response for computer generated microstructures with 20% elliptical Si particles in Al-Si-Mg matrix.
Figure 6.20: Damage configurations for RME $EH$ at (a) $\varepsilon_{xx} = 0.6\%$ (b) $\varepsilon_{xx} = 1.2\%$ and (c) $\varepsilon_{xx} = 2.0\%$

Figure 6.21: Damage configurations for RME $ER$ at (a) $\varepsilon_{xx} = 0.6\%$ (b) $\varepsilon_{xx} = 1.2\%$ and (c) $\varepsilon_{xx} = 2.0\%$
Figure 6.22: Damage configurations for RME RR at (a) $\varepsilon_{xx} = 0.6\%$ (b) $\varepsilon_{xx} = 1.2\%$ and (c) $\varepsilon_{xx} = 2.0\%$.

Figure 6.23: Effective plastic strain(%) for RME EH at (a) $\varepsilon_{xx} = 1.2\%$ and (b) $\varepsilon_{xx} = 2.0\%$.
Figure 6.24: Effective plastic strain (%) for RME ER at (a) $\varepsilon_{xx} = 1.2\%$ and (b) $\varepsilon_{xx} = 2.0\%$.

Figure 6.25: Effective plastic strain (%) for RME RR at (a) $\varepsilon_{xx} = 1.2\%$ and (b) $\varepsilon_{xx} = 2.0\%$. 
remaining relatively unstrained. This phenomenon is further accentuated with disparity in shapes, as can be seen for RME $RR$ in figure (6.25). Thus, models derived from a single damage parameter of simple microstructures can provide incomplete information of failure mechanisms in random microstructures. It is also important to note that strain levels in the microstructure of all 3 RMEs show no continuous matrix damage pattern, indicating clustering as the more predominant morphological factor influencing matrix failure.

Mark correlation functions of damage indicators (a) principal stress ratio in the particles through parameter $R_{ps}$ and (b) average plastic strain in the voronoi cell at various sampling distances $r$ are shown respectively in figures (6.26 a and b). Among
Figure 6.27: (a) Second Order intensity function and (b) Pair distribution function of relative orientation between elliptical particles in RME ER

Figure 6.28: Mark correlation function of (a) ratio of maximum principal stress to critical failure stress ($\sigma_{cr}$) (b) average effective plastic strain in each Voronoi cell with relative change in orientation of particles for RME ER
Figure 6.29: (a) Second order intensity function and (b) pair distribution function of relative change in form factor between elliptical particles in RME RR

Figure 6.30: Mark correlation function of (a) ratio of maximum principal stress to critical failure stress ($\sigma_{cr}$) (b) average effective plastic strain in each Voronoi cell with relative change in form factor of particles for RME $RR$
the 3 distributions, RME EH with particles of fixed shape and horizontal orientation, most closely resembles the uniform distribution. With the introduction of randomness in orientation, the mark correlation function of both damage indicators for RME ER show much slower attenuation with sampling distance $r$. This in turn underlines the need for larger window sizes to effectively represent morphological effects introduced by orientation. Disparity in the shapes of particles in RME RR, result in the greatest long range effect on the mark correlation function. While correlation of damage indicators with sampling distance $r$ provide qualitative information on the effect of shape/orientation on damage evolution, oscillation about the unit correlation of the uniform distribution suggest that $M(r)$ is an inefficient tool in measuring the actual morphological effect of these factors. In an attempt to provide a more descriptive function to study these factors, two alternatives to $M(r)$ are also implemented in this thesis. In the first, the relative orientation $\Delta \theta$ between particles is used to generate a second order intensity function $K(\Delta \theta)$ similar to the one outlined for sampling distance $r$. It is defined as the average number of additional particles that are oriented at an angle no greater than $\Delta \theta$ relative to a given particle in the microstructure. The second order intensity functions $K(\Delta \theta)$ and the corresponding pair distribution function $g(\Delta \theta) = \frac{dK(\Delta \theta)}{d\Delta \theta}$ for particles in RME ER, are shown respectively in figures (6.27 a and b). However, the resulting mark correlation functions $M(\Delta \theta)$ for the two damage indicators, shown in figure (6.28), continue to oscillate about the unit correlation produced by an uniform distribution. This is probably because relative orientation alone cannot account for the predominant morphological factor, viz. particle proximity, influencing damage evolution. Thus the effect of orientation on damage evolution needs to be modeled using a combination of these two
factors, i.e. by first quantifying the effect of orientation of particles in bringing them closer to each other and subsequently studying the clustering effect induced by the orientational distribution of particles. The morphological effect of shape is studied in a similar manner for RME \( RR S \). The relative change in form factors \( \Delta F \) between particles is used to generate a second order intensity \( K(\Delta F) \) and a corresponding pair distribution function \( g(\Delta F) \) which are shown respectively in figures (6.29 a and b). The resulting mark correlation function \( M(\Delta F) \), shown in figure (6.30), indicate a more pronounced influence of relative change in form factor on damage evolution in the microstructure. Influence of both damage indicators indicate disparity in particle shape tends to facilitate failure of the particles and the matrix of the RME.
Another important factor influencing damage evolution in random heterogeneous media is the size of the particles. While a more detailed discussion of size effects are provided in the following section, an introduction to its influence is carried out in this example. The critical stress to failure $\sigma_{cr}$, for particles in RME $RR$ is taken to be a geometric/material property, so that the competing effects shape and size on damage can be illustrated. The critical stress intensity $K_{IC}$ for the Si particles are calculated by back substituting $\sigma_{cr} = 300\text{MPa}$ along with the size of the particle in RME $EH$ onto the equation $K_{IC} = \sigma_{cr}\sqrt{\pi R}$. The resulting macroscopic response of RME $RR$, marked as $RR.S$, is shown figure (6.19). Damage evolution in the particles and the resulting growth of plastic strains in the matrix regions of the microstructure are shown respectively in figures (6.31 and 6.32). As expected, figure (6.31) indicate
that larger particles tend to fracture more easily when $\sigma_{cr}$ is taken to be geometric/material property. Many of the smaller particles remain undamaged even towards the end of the loading, resulting in a much larger load carrying capacity for the RME $RR_{RS}$ when compared RME $RR$. Evolution of plastic straining in the matrix material, indicate matrix failure originating between larger particles and traveling to other regions in the microstructure. It should be noted that the relative larger strains for much of the matrix material, when compared with RME $RR$ in figure (6.25), is due to the larger macroscopic load carried by the RME rather than due to fracture in the particles. The various morphological factors considered in this section could be isolated by artificially simulating the required microstructure with a predominant geometric pattern. However, in actual materials, all these factors maybe prevalent in the microstructure. The combined effect of the various morphological factors considered in this sections are used for the analysis of damage in actual microstructures considered next.

6.3 Modeling Damage from Actual Micrographs

In this concluding example, micrographs obtained from detailed serial sectioning of reinforced Al-Si-Mg alloys containing $\approx 10\%$ and $20\%$ by volume of Si particulates is simulated for damage evolution. The material is developed by ALCOA Technical Center by rapid solidification of fine powders using a gas atomization process [49], to achieve equiaxed Si particles. The powder is consolidated by cold isostatic compaction and then canned and degassed at 454°C for 6 hours. It is finally consolidated to full density by hot isostatic pressing in an extrusion press against a blind die.
Two types of microstructure are considered in this study, viz. (a) a naturally aged 20% volume fraction composite with with mean Si particle size of 4.4 μm, and (b) a naturally aged 10% volume fraction composite with with mean Si particle size of 3.6 μm. A serial-sectioning technique is performed to obtain a series of 2-D. The method involves gradual removal of material layers to obtain a series of optical micrographs representing sections of a composite microstructure, which are then digitized.

An equivalent microstructure (like in figure 6.33b) is first constructed by equating moments of the actual inclusion topology with those for equivalent ellipses used in the VCFE analysis. For the 0th, 1st and 2nd moments of the inclusion domain $\Omega^e$, the procedure results in the 5 equations:

\[
\begin{align*}
I_{00} &= \int_{\Omega^e} dx \, dy = \pi ab \\
I_{10} &= \int_{\Omega^e} y \, dx \, dy = y_c \pi ab \\
I_{01} &= \int_{\Omega^e} x \, dx \, dy = x_c \pi ab \\
I_{20} &= \int_{\Omega^e} y^2 \, dx \, dy = \frac{1}{8} \pi ab \{(a^2 + b^2) + (b^2 - a^2) \cos 2\theta\} + \pi ab y_c^2 \\
I_{02} &= \int_{\Omega^e} x^2 \, dx \, dy = \frac{1}{8} \pi ab \{(a^2 + b^2) - (b^2 - a^2) \cos 2\theta\} + \pi ab x_c^2 \\
I_{11} &= \int_{\Omega^e} xy \, dx \, dy = \frac{1}{8} \pi ab \{(a^2 - b^2) \sin 2\theta\} + \pi ab x_c y_c
\end{align*}
\]  

(6.2)

where $(x_c, y_c)$ is the centroid, $(a, b)$ is the principal axis and $\theta$ is the orientation of the equivalent elliptical inclusion. Equation (6.2) is solved simultaneously to obtain the geometric parameters $x_c, y_c, a, b,$ and $\theta$ for each of the equivalent inclusions. Optical micrographs, simulated equivalent microstructure and the tessellated voronoi cell meshes for the 4 RMEs considered in this example are shown in figures (6.33, 6.34, 6.35 and 6.36). Of these, the first two correspond to a volume fraction $V_f = 10\%$ of
Figure 6.33: (a) Optical Micrograph #1 of Al-Mg-Si Composite ($V_f = 10\%$) (b) Simulated Equivalent Microstructure (c) Tessellated Voronoi Cell Mesh
Figure 6.34: (a) Optical Micrograph #2 of Al-Mg-Si Composite ($V_f = 10\%$) (b) Simulated Equivalent Microstructure (c) Tessellated Voronoi Cell Mesh
Figure 6.35: (a) Optical Micrograph #3 of Al-Mg-Si Composite ($V_f = 20\%$) (b) Simulated Equivalent Microstructure (c) Tessellated Voronoi Cell Mesh
Figure 6.36: (a) Optical Micrograph #4 of Al-Mg-Si Composite ($V_f = 20\%$) (b) Simulated Equivalent Microstructure (c) Tessellated Voronoi Cell Mesh
Figure 6.37: (a,b) Particle size distribution for two sections of the actual Al-Si-Mg composite microstructure ($V_f = 20\%$).

Figure 6.38: (a,b) Cumulative distribution and probability density functions of local area fraction for two sections of the actual Al-Si-Mg composite microstructure ($V_f = 20\%$).
Figure 6.39: (a,b) Cumulative distribution and probability density functions of nearest neighbor distance for two sections of the actual Al-Si-Mg composite microstructure ($V_f = 20\%$).

Figure 6.40: (a,b) Second order intensity and pair distribution function for sampling radial distances in two sections of the actual Al-Si-Mg composite microstructure ($V_f = 20\%$).
Si particles in the composite and are denoted as #1 and #2. The last two correspond to a volume fraction of $V_f = 20\%$ and are denoted #3 and #4. For the $V_f = 10\%$ case, the equivalent microstructures #1 and #2 are made up respectively of 77 and 89 Si particles. The microstructures #3 and #4 for the $V_f = 20\%$ case consist respectively of 97 and 106 Si particles. Since the fracture of Si particles are modeled as a geometric/material property, the actual value of their effective diameters is critical in determining the onset of damage in the microstructure. The average effective diameter of $D_{avg} = 3.6\mu$ and $D_{avg} = 4.4\mu$ for the two volume fractions used in the analysis is obtained from image analysis performed by Kiser et.al.[50] for similar composite systems. The two dimensional area fraction for the microstructures are calculated to be $\approx A_f = 8.7\% and 18.6\%$ (note that the 3-D VF $\approx 10\% and 20\%$) and the microstructural representative material elements have dimensions of 228$\mu \times 180 \mu$ and 205$\mu \times 137 \mu$. 

Figure 6.41: (a,b) Second order intensity and pair distribution function for form factor in two sections of the actual Al-Si-Mg composite microstructure ($V_f = 20\%$)
While relevant results are presented for both volume fractions, the observed phenomena is explained predominantly respect to the 20% microstructures (i.e. \# 3 and \# 4). The distribution of effective particle diameter \( D \) for microstructures \# 3 and \# 4 is shown in figure (6.37). Considerable scatter of particle size and difference between the sections are observed in these figures. Cumulative and probability density distribution functions of the local area fraction and near-neighbor distance are plotted respectively in figures (6.38 and 6.39). They indicate a fairly uniform morphological distribution of particles for both sections. The second order intensity function \( K(r) \) along with its derivative, the pair distribution function \( g(r) \) is used to quantify clustering, if any, of particles in the microstructures. Figure (6.40), depict the resulting spatial distribution of particles for the two sections, indicating little or no clustering of particles in either section. Shape effects on damage of the microstructure is studied through the second order intensity function \( K(\Delta F) \) developed in the previous section. Figure (6.41) exhibit this function along with its derivative \( g(\Delta F) \) for the two sections. When compared to the pair distribution functions for RME RR in figure (6.29), the actual micrographs exhibit a larger disparity between shapes of particles. The maximum observed form factor at either volume fraction is 0.97 and the minimum observed value is 0.48.

As in the previous examples, the deformations in the matrix material of undamaged voronoi cells is modeled using 34 stress coefficients (25 polynomial + 9 inclusion based reciprocal terms ) and those in the damaged voronoi cell are modeled using 70 stress coefficients (25 polynomial + 9 inclusion based reciprocal terms + 36 crack based reciprocal terms). The corresponding inclusion deformations of the undamaged
Figure 6.42: Macroscopic compressive stress-strain response for the Al-Si-Mg composite specimens at two volume fractions.

Voronoi cells are modeled using 25 stress coefficients (25 polynomial terms) and those of the damaged voronoi cell are modeled using 61 stress coefficients (25 polynomial + 36 crack based reciprocal terms). The material properties of the constituents are as follows:

**Al-Mg Matrix**

Young's Modulus $E = 69$ GPa, Poisson's Ratio $\nu = 0.33$

Post yield behavior (Non-linear isotropic hardening) Digitized from data in Kiser et al. [50].

**Si Inclusions**

Young's Modulus $E = 161$ GPa, Poisson's Ratio $\nu = 0.2$

Mode I Critical Stress Intensity Factor $K_{IC} = 0.6$ MPa$\sqrt{m}$
Figure 6.43: Probability of failure of Si particles as a function of (a) particle area and (b) particle principal stresses.

In order to study the undamaged behavior of the 4 RMEs, they are loaded compressively to macroscopic tensile strain of $\varepsilon_{xx} = 6\%$. The resulting macroscopic response, shown in figure (6.42), indicate that the $V_f = 20\%$ composite has a stiffer response when compared to the $V_f = 20\%$ composite. For damage analysis, the microstructures are loaded in uniaxial tension along the horizontal direction to a macroscopic strain of $\varepsilon_{xx} = 6\%$ under plain strain conditions.

In order to analyze damage evolution in the RMEs, the initial flaw size in the particles is assumed to be $c = 0.125 D$. The critical stress to fracture for individual particles is modeled using the fracture mechanics based criterion $\sigma_{cr} = \frac{Kc}{\sqrt{a c}}$. The choice of initial flaw size tends to be empirical and its rationale is provided in the following paragraph. At the beginning of the loading process, initial flaw sizes in
Figure 6.44: Actual micrographs for 10% Al-Si-Mg composite at $\varepsilon_{xx} = 3\%$ for (a) Microstructure #1 and (b) Microstructure #2.

Figure 6.45: Actual micrographs for 20% Al-Si-Mg composite at $\varepsilon_{xx} = 6\%$ for (a) Microstructure #3 and (b) Microstructure #4.
Figure 6.46: (a,b) Histograms of number of damaged particles at $\varepsilon_{yy} = 6\%$, by Weibull distribution and fracture mechanics based damage criteria respectively.

...individual particles are unavailable. Further, due to the destructive nature of SEM, experimental data of individual particle fracture is usually available at exactly one macroscopic strain level. Consequently an estimate of the flaw size is performed based on their ability to reflect actual microstructural damage as well as their ability to model the resulting macroscopic deformations. In this example, flaw sizes were estimated based on analysis performed on an auxiliary RME (not shown here). The fraction $e = c/D = 12.5\%$ was obtained based on (a) accurate depiction of actual particle failure at the same overall strain level and (b) similar macroscopic behavior over the entire range of loading.

While individual strengths of the Si particles can be calculated from a simple fracture mechanics criterion, alternative statistical correlations linking particle size/stress...
levels to particle fracture are also commonly used to study damage in brittle/metal matrix composites. Curtin[86], Amornsukhai [87] and Kiser et.al.[50] have used the Weibull distribution to characterize the onset of particle fracture. In such a description, the probability of failure of a particle $\psi$ is related to its area $A$ and maximum principal stress $\sigma_I$ through the relation:

$$\psi = 1 - \exp - A\left(\frac{\sigma_I}{\sigma_{cr}}\right)^m$$  \hspace{1cm} (6.3)

where the Weibull parameters $\sigma_{cr}$ and $m$ are characteristics of the inclusion material. Consequently, damage in individual particles increases with the presence of larger particles and at larger load levels. Weibull parameters $\sigma_{cr}$ and $m$ for the Si material are calculated by correlating stress levels/particle areas with damage from the actual micrographs. In order for such a method to work, micrographs at the onset of particle cracking should be available. Micrographs for the 10% microstructures # 1 and # 2 at a macroscopic tensile strain of $\varepsilon_{xx}$ = 3%, shown in figure (6.44), exhibit these properties and are hence used for calculating the the weibull parameters. In this procedure, areas $A$ of individual particles are obtained through scanning of the optical micrographs and VCFE analysis of RMEs (with no damage in the microstructure) at a macroscopic tensile strain of $\varepsilon_{xx}$ = 3% are used to predict microscopic stress levels $\sigma_I$ in each of the particles. Damaged particles from the actual micrographs are assumed to have a large probability of failure $\psi > 0.95$, and a non linear least square fit of $\psi(m, \sigma_{cr})$ of damaged particles, is used to derive the the Weibull parameters. For the Al-Si-Mg composite considered in this example, the probability of damage in the Si-Particles is obtained through the parameters $m = 2.37$ and $\sigma_{cr} = 2.12$ GPa. In the above, the value of $\sigma_{cr} = 2.12$ GPa corresponds to area units $\mu^2$ and alternative units for the particle area would alter only $\sigma_{cr}$. The probability of failure of individual
Figure 6.47: Macroscopic tensile stress-strain response for the Al-Si-Mg composite specimens at two volume fractions

particles $\psi$ as a function of particle area and stress levels, are shown respectively in figures (6.43a and b). They indicate that both larger particles at lower microscopic stress levels and smaller particles at higher microscopic stress levels contribute towards microstructure failure.

In order to ascertain the accuracy of the two damage criteria, the damage levels generated by VCFEM for microstructure # 3 is compared with those obtained from the actual micrograph (see figure 6.45a) at a macroscopic tensile strain of $\varepsilon_{xx} = 6\%$. The resulting histograms for the fraction of cracked particles of given size is shown in figure (6.46). The plots indicate that a while both damage criteria are effective in simulating fracture of larger particles, the Weibull distribution based damage criterion

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Figure 6.48: Simulated configurations of evolving damage at (a) $\varepsilon_{xx} = 3.0\%$, (b) $\varepsilon_{xx} = 4.2\%$ and (c) $\varepsilon_{xx} = 6.0\%$ with a Weibull distribution based damage criterion provides a more accurate depiction of damage levels in smaller particles. Consequently the Weibull distribution is used as the damage criterion to analyze the failure of all the microstructures.

The resulting macroscopic tensile response of the Al-Si-Mg composite at both volume fractions is shown in figure (6.47). These plots also show the overall stress-strain response of an idealized microstructure with a single circular inclusion with the same average diameter. It can be seen that the single inclusion does not fail for the $V_f = 10\%$ RME and consequently predicts a much stiffer response than that of the random microstructure. For the $V_f = 20\%$, abrupt failure of the single particle results in an overestimated value for the damage level $\rho = 100\%$, resulting in a much larger drop in the load carrying capacity of the RME. On the other hand, VCFEM results
Figure 6.49: Contour plots of probability of failure in undamaged particles for microstructure # 1 from a Weibull based damage criterion immediately before (a) $\varepsilon_{xx} = 4.2\%$ and (b) $\varepsilon_{xx} = 6.0\%$. (Damaged particles are shown with the cracks)

Figure 6.50: Effective plastic strain (%) contours for microstructure # 1 after (a) $\varepsilon_{xx} = 4.2\%$ and (b) $\varepsilon_{xx} = 6.0\%$. 

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Figure 6.51: Contour plots of probability of failure in undamaged particles for microstructure # 3 from a Weibull based damage criterion immediately before (a) $\varepsilon_{xx} = 4.2\%$ and (b) $\varepsilon_{xx} = 6.0\%$. (Damaged particles are shown with the cracks)

Figure 6.52: Effective plastic strain (%) contours for microstructure # 3 after (a) $\varepsilon_{xx} = 4.2\%$ and (b) $\varepsilon_{xx} = 6.0\%$. 

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for the actual microstructures provide a good description of the macroscopic response of the composite at both volume fractions, although the simulated load carrying capacity is stiffer at both volume fractions. The higher values are attributed to the 2-d small deformation analysis carried out by VCFEM as opposed to the more realistic 3-d large deformations undergone by the actual microstructure. Another source of error in the current model is the absence of matrix damage which is expected to lower the load carrying capacity of the composite. It is also interesting to note, that at both volume fractions, VCFEM response is very similar to experimental results. The crossover point, when the 20% composite becomes less stronger than the 10% composite, is around $\varepsilon_{xx} \sim 1.2 - 1.8\%$ by the current analysis and compares well with the experimental value of $\varepsilon_{xx} \approx 1.8\%$. Progressive fracture of individual particles for all RME $\# 3$ is shown in figure (6.48). As expected, the damage in the microstructure
is initiated by fracture of larger particles, with a large number of the smaller particles remaining undamaged at the end of the loading.

The distribution of probability of failure and plastic strains for microstructures #1 at various stages of the loading are shown respectively in figures (6.49 and 6.50). Probabilities of failure, shown only for undamaged particles, depicts future sites of damage in the microstructure. At the beginning of the load increment leading to a tensile strain of $\varepsilon_{xx} = 4.2\%$, a few of the larger particles in the microstructure appear as possible sites of damage (i.e. $\psi > 0.95$). However with continued loading, as can be seen from figure (6.49 b), some of these particles remain intact until the final loading increment. Failure of neighboring particles have thus prevented further loading of some of the particles that were close to failure at a $\varepsilon_{xx} = 4.2\%$. This phenomenon, which was also apparent in the particle clustering example, indicates evolving microstructural morphology in damaging materials can considerably influence future sites of damage. The plastic strain distribution in figure (6.50 a) indicate severe localization is restricted to small areas of the microstructure, with no well defined pattern to suggest complete failure of the material. As can be seen from figure (6.50 b), continued loading results in a fairly uniform straining of the matrix material, with most parts of the RME exhibiting plastic strains $\approx \varepsilon_{xx} = 6\%$.

The corresponding probabilities of failure and plastic strain distributions for microstructure #3 is shown in figures (6.51 and 6.52). Once again, a comparison of principal stress distributions among the undamaged particles in figures (6.51 a and
b) indicate that particles that are near failure need not necessarily fail upon subsequent loading. The plastic strain distribution in figure (6.52 a) indicates severely localized deformations forming a more continuous pattern than in microstructure #1. It can also be seen that the remainder of the matrix undergoing much smaller deformations, suggesting matrix failure along these bands. Figure (6.52 b) shows that continued loading has resulted in severe degradation of the microstructure. Experimental results indicated failure of the 20% composite at a macroscopic tensile strain of $\varepsilon_{xx} = 6\%$.

While the current model does not allow directly for matrix failure, many traditional methods have used a porous description of the matrix material to model onset of softening in the microstructures. Tvergaard[19], Needleman[21, 20], and Finot
et.al.[47] use the Gurson-Tvergaard constitutive equations to derive the microscopic non-linear stress-strain response of the ductile matrices. The associated yield function exhibits an elastic-plastic response for both deviatoric and hydrostatic loading with the latter providing for the softening behavior in the matrix. The pressure distribution in the matrix, is therefore a good indication for possible sites of failure in the matrix. Evolution in the pressure distribution of RME # 3 is shown in figure (6.53). They indicate large pressure fields developing between cracks, signalling possible sites of localized matrix softening. When coupled to the corresponding plastic strain distribution in figure (6.52), the pressure distribution in the matrix indicate probable evolution paths for matrix crack which will ultimately combine into a macro-crack.
Mark correlation of the damage indicators for the 20% composite, with sampling distance $r$ is shown in figure (6.54). Both microstructure #3 and #4 depict show medium fluctuations at large sampling distances, indicating optimality in RME size w.r.t computational effort. Further, for both microstructures, the fluctuations are fairly uniform about the unit correlation, implying insignificant clustering effect at this volume fraction. On the other hand, mark correlation of the damage indicators with relative change in form factor, shown in figure (6.55), depict a positive correlation of damage with particle shape. Thus the damage analysis of actual microstructures, with a morphological distribution in the shape of particles, is essential to successfully predict failure in such materials.

6.4 Conclusions

VCFE simulations of evolving damage in random heterogeneous media are presented in this chapter. Simulated computer microstructures have been used to the study the stereological effects of various morphological characteristics, such as position shape and orientation, on the evolution of damage in the microstructure. Morphological distribution of particles to form clusters is shown to facilitate growth of damage of the microstructure. Disparity in shapes are also seen aid damage propagation in the material. Of the various factors analyzed in this chapter, effective statistical representations of damage for position and shape effects have been obtained through mark correlation functions. Statistical representation of orientation effects, however, remain unresolved in this work. The mark correlation functions generated in this thesis are also useful in predicting the length scales that may be required for accurate
material modeling. A comparison of the current model with experimental results demonstrate the ability of VCFEM to capture the many of the failure characteristics in actual materials. These include (a) reasonable match in macroscopic response (b) accurate simulation of damage in particles and (c) qualitative predictions on macro damage. However, the lack of a matrix failure model prevents a quantitative analysis of damage evolution from the particle onto the matrix and hence failure in the material. Statistical analysis for actual microstructures reveal that size and shape are the predominant factors influencing damage in these materials.
CONCLUSIONS AND FUTURE STUDIES

In this thesis, the Voronoi Cell Finite Element Method (VCFEM) has been developed for material modeling of damaged arbitrary heterogeneous media. The material based Voronoi cell mesh is generated using the Dirichlet Tessellation of the microstructure. The resulting 2 dimensional representative material element (RME) consists of Voronoi polygons containing a single heterogeneity. An assumed stress hybrid method is employed to analyze the elasto-plastic microscopic deformations undergone by the RME due to applied macroscopic loading. Damage in the microstructure is initiated through particle fracture triggered by the microscopic deformations in the heterogeneity. Consequently, evolving failure in the microstructure can be analyzed by the current scheme. The computational scheme allows for automatic generation of new topologies introduced by progressive failure of particles, and thereby avoids any user interference that might be required to rediscr etize the evolving microstructure.

Numerical validation of VCFEM is established in 2 stages. In the first stage, the VCFEM is compared with analytical and traditional computational methods for
undamaged media. Validation, in this stage, is performed for both simple and arbitrary microstructures. The simulations demonstrate VCFEM provides excellent comparisons of overall material properties with a very good representation of the actual microscopic stress/deformation fields. In the second stage, the current scheme is compared with traditional finite element schemes for simple microstructures. Once again, the VCFEM results produce a very good representation of both macro/microscopic properties of the material. Damage in arbitrary heterogeneous media, however, cannot be analyzed by most computational/analytical schemes. Further, experimental data available at the microstructural level tends to be restricted to discrete time intervals with only limited microscopic information available for comparison. Consequently, the VCFEM for arbitrary heterogeneous media is validated indirectly (i.e. with secondary variables such as extent of particle fracture, overall response of different morphological distributions) with experimental results. While these simulations provide a favorable comparison, several issues pertaining to the validity of the model remain unresolved. Some of these issues include (a) validity of the damage criterion used in the current analysis, (b) effect of matrix failure on the damage and response of the material (c) effectiveness of the current model to represent deformations in actual microstructures. Of these, the first two issues need to be investigated in greater detail. Possible avenues of exploration include (a) modification of current damage initiation model from a critical stress based to a critical energy based approach (b) inclusion of micro void growth into the matrix constitutive response to model failure propagation into the matrix. The third issue, pertaining to validity of the current scheme in representing actual microscopic deformations can be resolved if and when better experimental simulations of such materials is possible. Efforts in this regard
made by Davidson[51] and Majumdar et.al.[52] show promising possibilities in the near future.

Effect of morphological distributions on the damage of arbitrary heterogeneous materials has also been studied in this work. Some of the important features analyzed in the study include (a) required length scale at which microstructural analysis needs to be performed in order to effectively predict overall material properties (b) influence of proximity, shape and size of heterogeneities on damage in the microstructure. Statistical analysis of long range effects of damage in actual microstructure indicate a progressive increase of requisite length scales with evolving failure. This in turn implies that decoupling of macro/micro problem, as has been implemented by classical homogenization theories, may no longer be valid. Consequently, alternative methods such as direct interaction models, need to be used to simulate the deformations of damaging structural components. Shape and proximity have been shown to have a direct effect on the evolving damage of microstructures. While this finding is in agreement with many independent experimental studies, the effect of these morphological parameters on matrix failure seems to be underestimated. Modifications to the matrix constitutive laws, suggested in the previous paragraph, could help resolve this issue.

The VCFEM provides a direct interface for calculating material properties at various locations in a structure, which can than be used for the analysis of the structural deformations. Important advancements have been made by Ghosh & coworker[93, 94] in modeling elastic/elasto-plastic structural deformations with underlying random undamaged microstructures. Issues pertaining to failure in structures are also currently
under investigations. While the primary motivation of the study was to successfully model damage in random heterogeneous media, effective implementation of the computational scheme along with a coupled structural analysis demands a considerable amount of work dedicated towards the optimization of the computer program. An important accomplishments in this regard is the single processor optimization of the code on both vector (CRAY-YMP) and scalar (SUN-SPARC20) machines. A direct comparison with traditional finite element models for undamaged random media show a factor of saving of ~ 30-50. A similar comparison could also be seen for damage in simpler microstructural representations. Coupled with the modeling time, which would be far greater for traditional finite element methods, the VCFEM shows excellent prospects as an alternative material modeling tool.
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