Mesoscopic simulation of grain boundary diffusion creep in inhomogeneous microstructures

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MESOSCOPIC SIMULATION OF GRAIN BOUNDARY DIFFUSION CREEP IN INHOMOGENEOUS MICROSTRUCTURES

A Thesis

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Master of Science in Mechanical Engineering

in

The Department of Mechanical Engineering

By
Kanishk Rastogi
B.E., Punjab Engineering College, Panjab University, Chandigarh, India, 2002
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Dedication

Dedicated to my Nanaji, Mr. R. K. Rastogi,
For always being a source of inspiration and for his belief in me,
which has kept me firm.....always !!!
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Abstract

At high temperatures, stresses well below the material’s tensile yield strength can induce permanent deformation over a period of time. This time-dependent progressive deformation of a material at constant stress is called Creep and is observed in both crystalline and non-crystalline solids. The principal deformation processes contributing to creep deformation are slip, sub-grain formation and grain-boundary sliding. Mechanisms involving creep of crystalline materials involve either dislocation motion or diffusional flow of atoms or both. Extensive studies have been done to ascertain the creep mechanism in various regimes of temperature and applied stresses. At low stresses and high temperatures, grain boundary sliding accommodated diffusion creep i.e. Coble creep is the dominating mechanism. Apart from the experimental investigations, various analytical models have been proposed to explain the underlying principles of this process. However, these studies have been limited to small idealized microstructures. Computational models involving complex mathematical formulations have been developed to study Coble creep in homogeneous microstructures.

The present study is to investigate the effect of microstructural inhomogeneity on the stress concentrations in the microstructure and the strain rate. These stress concentrations at grain boundaries arising from microstructural inhomogeneity affect the mechanical properties of polycrystalline materials. Moreover, since the strain rate in Coble creep is dependent on grain size, it is imperative to study the strain-rates in inhomogeneous microstructures to get a realistic idea of the deformation process. Our simulation results indicate that not only creep rate is lowered by the presence of inhomogeneities, but the stress concentrations are also significantly altered giving rise to tensile stresses as high as three times the external applied stress on the system.
1. Introduction

1.1 General

Creep is the continuing plastic deformation of materials subjected to a constant load or constant stress [1]. The engineering creep properties of a metal can be determined by applying a constant load to a tensile specimen maintained at a constant temperature, and the strain of the specimen is determined as a function of time [2]. Results from experimental and theoretical studies have established that the creep of crystalline solids occurs as the result of thermally-activated migration of dislocation, grain-boundary diffusion and shearing, and diffusion of vacancies. It can take place at all temperatures above absolute zero [1]. The chief creep deformation mechanisms have been grouped as, dislocation glide (thermally activated dislocation motion along slip planes at high stresses); dislocation creep (dislocation motion by thermally assisted mechanisms involving vacancy/interstitial diffusion at intermediate stresses); diffusion creep (vacancy/interstitial flow through a crystal under low stresses) and grain boundary sliding (sliding of grains past each other) [2].

High-temperature alloys find applications in a wide variety of applications and their selection depends on factors like application temperatures, stress-levels and engineering requirements. Typical applications include furnace parts, piping, steam turbine rotors, boiler tubes, superheater tubes (moderate temperatures, upto 550 °C); heat exchangers, boiler baffles, furnace linings, jet-engine burner liners, exhaust systems for gas turbines (high temperatures, upto 1000 °C) and aircraft gas turbine engines (more than 1100 °C). Various studies of the creep phenomenon and its underlying mechanisms have pointed to the importance of diffusional creep at most of the stress-levels and temperature ranges in the engineering applications [3, 7].
Fine-grained materials (< 10 µm) exhibit a phenomenon of superplasticity which is closely related to creep. Superplasticity refers to a phenomenon in which certain materials subjected to high temperature demonstrate remarkably high strains to failure. Superplastic materials exhibit a strong strain-rate dependence of the flow stress over a limited temperature range and in this range they are capable of extensive uniform plastic deformation. Superplastic deformation has important industrial applications like high-temperature forming of complex shapes of inherently brittle materials like ceramics and intermetallics [1, 3, 4]. Superplastic deformation has been studied for materials like Pb-Sn, Zn-Al, Cd-Zn eutectics, mechanically alloyed aluminum, SiC-reinforced Al composites, nickel aluminides and Y-TZP ceramics. These studies are focused on the flow properties of these materials, strain-rate dependence and failure [25]. Characteristics of superplastic materials include a fine-grained equiaxed microstructure (grain size < 10 µm) and resistance to grain growth at temperatures and time duration of superplastic deformation. Another microstructural feature of superplastic deformation is that grain shape is essentially preserved during the deformation [3, 4]. Fundamental studies to ascertain the mechanism of superplasticity have pointed to the diffusional creep and extensive grain-boundary sliding.

A lot of fundamental and theoretical studies have been done so far to ascertain the mechanism behind diffusional creep and grain-boundary sliding. Analytical models have been proposed by Ashby [33], Spingarn [36], Hazzledine [39], Gifkins [49] and Langdon[55-56] on small uniform grain arrangements showing various modes of diffusion and accommodating grain-boundary sliding. However, since the real systems are large and quite complex to model analytically, computer simulations are used as a valuable tool in modeling them. Pan and Cocks [42] first proposed a simulation methodology for the diffusion creep phenomenon.
using finite-element approach. Hazzeldiene [39] formulated a theory for the small irregular grain structures (25 grains) containing single large grain. However, using the available computational sources, there still exists a need to simulate large grain structures containing microstructural inhomogeneities, so that the theoretical predictions can be used to apply in the real applications. The present study focuses on this aspect using mesoscale simulations and is an extension of the work done by Moldovan et al [50] in grain-boundary diffusion controlled creep.

1.2 Objective

The objective of this work is to study the:

(a) effect of microstructural inhomogeneity on the overall deformation mechanism by grain-boundary diffusion creep.

(b) stress distribution in a system containing microstructural inhomogeneity.
2. Background and Literature Review

2.1 Review of Creep Phenomenon

At high temperatures, stresses well below the material’s tensile yield strength can induce permanent deformation over a period of time. This time-dependent progressive deformation of a material at constant stress is called creep and is observed in both crystalline and non-crystalline solids. Mechanisms involving creep of crystalline materials involve dislocation motion or diffusional flow of atoms [3]. The engineering creep curve of a material can be determined by applying a constant load to a tensile specimen maintained at constant temperature, and the strain of the specimen is determined as a function of time. This is called constant-load creep test. In engineering applications, load is usually maintained constant and hence creep curve can be used to determine the high-temperature properties of a material. Fundamental studies of the creep mechanism are carried under constant-stress conditions [2]. Figure 2.1 illustrates schematically the creep behavior of a material subjected to a constant true stress [3]. The slope of this curve refers to as the creep rate ($\dot{\varepsilon} = d\varepsilon / dt$). This creep curve can be divided into three stages: instantaneous elongation followed by decelerating primary creep, a linear portion designated as secondary creep and finally accelerated creep, followed by fracture.

The first stage, known as primary creep, represents a region of decreasing creep rate. It is a period of transient creep in which the creep resistance of the material increases by virtue of its own deformation. This is similar to the work-hardening in metals at lower temperatures e.g. dislocation density increases and a dislocation subgrain structure is formed with a cell size that decreases the strain. For low temperature and stresses, primary creep is the predominant creep process. The second stage of creep, known as secondary creep, is a period of nearly
constant creep rate which results from a balance between the competing process of strain hardening and recovery. If recovery processes are not concurrent with deformation then dislocation density would increase and a subgrain structure would become progressively finer with increasing strain. Hence, hardening mechanisms effective at low temperature are not as effective at higher temperature. Microscopically, it can be said that the nonconservative dislocation motion renders obstacles to glide less effective at elevated temperatures and also dislocations are removed from the material simultaneously by recovery. This is also referred as steady-state creep. The average value of creep rate during secondary creep is called the minimum creep rate. Third stage is known as tertiary creep. During this stage, the creep rate exceeds that of secondary creep and increases continuously leading to fracture. Transition from second stage to third stage can be attributed to several microscopic changes in the material like onset of recrystallization, coarsening of precipitate particles and the formation of internal crack or voids. These internal cracks and voids are precursors to fracture.

Figure 2.1: A typical creep curve showing the three stages of creep [3].
The secondary stage is most important in determining the creep properties of any materials. A material’s engineering creep resistance is characterized by one or both of the parameters \( \dot{\varepsilon}_H \) (steady-state creep rate) and \( t_f \) (time to fracture). They represent extreme design criteria. Fundamental discussions for creep mechanism consider only \( \dot{\varepsilon}_H \). In applications where secondary creep constitutes a significant portion of material’s total strain, \( \dot{\varepsilon}_H \) and \( t_f \) are inversely related. For example, in short-time elevated temperature use (“one shot rocket engine component”), creep deformation may be tolerable but fracture is not. Thus here, \( t_f \) is an appropriate design parameter. For components designed for high-temperature operation for hundreds to thousands of hours (jet engine turbine blade or boiler tubing), structural integrity is required i.e. low permanent strain. Hence, \( \dot{\varepsilon}_H \) is critical design parameter in such applications [1 - 3].

Figure 2.2 shows the effect of applied stress (temperature) on the creep curve at constant temperature (stress). It can be observed that the creep curve with three well-defined stages can be found only for certain combinations of stress and temperature. Similar trend can be seen in

![Figure 2.2](image)

Figure 2.2: Schematic representation of the effect of increasing stress (temperature) keeping temperature (stress) constant [2].
a family of curves obtained for creep at constant stress for different temperatures. The higher the temperature, the greater the creep rate [2, 3,7].

The steady state creep rate can be correlated to applied stress and temperature by an equation of the form:

\[
\dot{\varepsilon}_\tau = A\sigma^m \exp \left[ \frac{-Q_C}{RT} \right]
\]  

(1)

where A and m are constants and Q_C is the creep activation energy. Equation (1) can be applied over a limited stress/temperature range as the constants A, m and Q_C vary with stress and temperature. These variations lead to change in creep mechanisms [3].

2.2 Creep Mechanisms

Inhomogeneities play a significant role in high-temperature deformation. The principal deformation processes are slip, sub-grain formation and grain-boundary sliding. Secondary deformation processes include multiple slip, formation of extremely coarse slip bands, kink bands; fold formation at grain boundaries, and grain boundary migration. New slip systems become active at elevated temperatures and slip occurs on many planes for small slip distances. Dislocation loops climb and annihilate each other resulting in steady stream of dislocations. Inhomogeneous creep deformation results in lattice bending near grain boundaries generating excess dislocations of one sign. These dislocations climb readily at high temperature and arrange themselves into a low angle grain boundary, thus forming a subgrain structure within a grain. Another important structural change is grain boundary sliding. At elevated temperature the grains in a polycrystalline metals are able to move relative to each other. Grain boundary sliding is a shear process which occurs along a grain boundary. It is enhanced by increasing the temperature and/or decreasing the strain rate when
void nucleation and coalescence is delayed. Sliding becomes prevalent and wedge cracks and voids grow on the grain boundaries lying roughly normal to the tensile axis [1 - 4].

The flow stress \( \sigma \) (i.e. the stress to cause plastic flow), can be described as a function of strain rate, \( \dot{\varepsilon} \), and absolute temperature, \( T \), in the form [5]:

\[
\dot{\varepsilon} = A \frac{DGb}{kT} \left( \frac{\sigma}{G} \right)^n
\]  

(2)

where \( D \) is the diffusion coefficient, \( k \) is the Boltzmann’s constant, \( n \) is the stress exponent, \( G \) is shear modulus, \( b \) is Burger’s vector, and \( A \) is a function of microstructure (reflecting the influences of grain size, subgrain size and dislocation density). Grain size effect can be included in the modified equation:

\[
\dot{\varepsilon} = A \frac{DGb}{kT} \left( \frac{b}{d} \right)^p \left( \frac{\sigma}{G} \right)^n
\]  

(3)

where \( d \) is the grain size and \( p \) is a constant. Equation (3) is called power law equation and has the empirical values of \( n \), \( p \) and \( D \) for different creep mechanisms. Since diffusion coefficient can be described as:

\[
D = D_o \exp \left[ \frac{-Q_c}{RT} \right]
\]  

(4)

equation (3) can be rearranged in a form similar to equation (1) [2,4]:

\[
\dot{\varepsilon} = B \sigma^n \exp \left[ \frac{-Q_c}{RT} \right]
\]  

(5)

where \( B \) is a constant.
2.2.1 Dislocation Creep

Dislocation creep refers to deformation controlled by dislocation slip in grain lattice as shown schematically in Figure 2.3. The slip process involves both glide on slip planes and climb over physical obstacles.

At low stresses ($\sim \sigma/G < 10^{-6}$), a linear dependence on stress is observed i.e. $n=1$ and this is known as Harper-Dorn creep [8]. This is governed by climb-controlled dislocation motion in the grain interiors without affecting the dislocation density with stress. It does not depend on grain size. At intermediate stresses, power-law creep is observed with:

\[ n = 3 \text{ for solid solution} \]
\[ n = 4-5 \text{ for pure metals} \]

In solid-solutions, creep is controlled by the glide step in glide/climb mechanism as solute atoms resist dislocation motion. Creep rate is given by [9]:

\[ \dot{\varepsilon} = KD_s\sigma^3 \]  

where $D_s$ is the diffusion coefficient of solute atom in the alloy.

Figure 2.3: Schematic illustration of dislocation creep involving both climb and glide of dislocations [4].
In pure metals dislocation climb requires more energy than glide and thus creep deformation is controlled by climb of dislocations over physical obstacles. Figure 2.4 represents such a process. Creep rate is given by [10]:

\[ \dot{\varepsilon} = K D_L \sigma^n \]  

(7)

where \( D_L \) is lattice diffusion coefficient and \( n = 4-5 \).

At high stresses (\( \sim \sigma / G > 10^{-3} \)), simple power law fails as measured strain rates are greater than that it predicts. The process is now a glide-controlled flow instead of climb-controlled (Figure 2.5). Combined rate equation for power-law creep and power-law breakdown can be given by the empirical relation [11]:

\[ \dot{\varepsilon} = A \frac{D G b}{\alpha^a k T} \left[ \sinh \left( \frac{\alpha \sigma}{G} \right) \right]^a \]  

(9)

Figure 2.4: Power law creep involving cell formation by climb [6].

Figure 2.5: Power law breakdown. Dislocation glide controls the process [6].
At very high temperatures (≥ 0.7 T_M), power-law creep is accompanied by dynamic recrystallization, changing the dislocation substructure by inducing new regimes of primary creep in newly formed grains, thus drastically increasing the strain rates [1, 4, 6, 7]. Schematic illustration is shown in Figure 2.6.

2.2.2 Diffusion Creep

At very low stress, dislocation motion is very negligible and slow and thus, can be ignored. Under such conditions, stress application on a polycrystalline material, results in an excess of vacancies along those grain boundaries experiencing tensile stress and a corresponding depletion of vacancies along those experiencing a compressive stress. Diffusion creep refers to the stress-directed flow of vacancies that takes place in order to restore an equilibrium condition. This flow of vacancies is equivalent to the flow of atoms in opposite direction and it leads to an elongation of the individual grains along the tensile axis (Figure 2.7). Thus the grains deform keeping the same neighbors, a characteristic of diffusion creep [12, 17].
Creep continues by diffusional flow i.e. the diffusive motion of atoms from sources on grain boundaries that carry a compressive load to sinks which carry a tensile load. This process is diffusion controlled and strain rate increases roughly linearly with stress. It occurs typically in fine grained materials at very high temperatures when atomic diffusion is rapid. The key idea is that boundaries allow deformation to occur solely by diffusional mass transport.

If the transport of matter is diffusion through the grain lattice (Figure 2.8), it is called Nebarro-Herring creep and rate equation is expressed as [13-14]:

$$
\dot{\varepsilon}_{NH} = A \left( \frac{D_L}{d^2} \right) \left( \frac{\sigma \Omega}{kT} \right)
$$  \hspace{1cm} (10)

where $\Omega$ is the atomic volume, $D_L$ is the lattice self-diffusion coefficient and $A \sim 10$ is a numerical factor depending mainly upon the shape of grains. The resulting change in grain dimensions after the diffusion of mass flux and vacancy flux through the bulk is equivalent to creep strain (Figure 2.8 b).
Coble creep is similar to Nabarro-Herring creep and is driven by vacancy concentration gradient. Mass transport occurs by diffusion along grain boundaries as shown in Figure 2.9. The diffusion area thus depends on the grain-boundary thickness. Expression for the creep is [15]:

\[
\dot{\varepsilon}_c = A \left( \frac{D_{GB} \delta'}{d^3} \right) \left( \frac{\sigma \Omega}{kT} \right)
\]

(11)

where \( D_{GB} \) represents grain-boundary diffusion coefficient, and \( \delta' \) is the grain-boundary thickness.

Figure 2.8: Schematic representation of Nabarro-Herring creep [4].

Figure 2.9: Schematic illustration of Coble creep where atomic flow occurs along the grain-boundaries of the hexagonal grain [4].
Coble creep ($\sim 1/d^3$) has a stronger dependence on grain size than Nabarro-Herring creep ($\sim 1/d^2$) and is thus more important in very fine grained materials. Also, the activation energy for grain-boundary diffusion is smaller than that for the lattice diffusion ($Q_{GB} \approx 0.6 Q_L$ approx). Creep by self-diffusion through the matrix i.e. Nabarro-Herring creep is predominant mechanism at low stresses and high temperatures. Coble creep is more important at low stresses and lower temperatures.

Even though dislocation creep and diffusional creep, both are thermally activated and depend on stress, volume and temperature in a similar way, but their activation energies and corresponding volume terms are remarkable different. Diffusion creep is important in superplastic deformation where it provides the high strain-rate sensitivity of the flow stress necessary for superplastic behavior [3, 4, 6, 7, 16, 17].

2.2.3 Grain Boundary Sliding

Grain boundary sliding (GBS) occurs during creep as grain boundaries are imperfectly bonded and thus weaker than the ordered crystalline structure of the grains. The regions close to the grain boundaries deform plastically at an applied stress much lower than that required to deform the interior because the stress concentrations at the intersections of the grain boundaries and at the curved portions of the grains cause local regions of the plastic strain [4]. It does not contribute significantly to the power-law creep and strain contributions by GBS are typically less than 0.2 of the total strains. Major contribution to strain is dislocation movement and GBS is controlled by the same dislocation climb processes which control the overall creep rate [17, 18]. However, at lower stresses, GBS becomes prevalent and helps in initiating intergranular fracture by facilitating wedge cracks and voids growth on the grain boundaries lying roughly normal to the tensile axis [2].
The superplastic behavior in fine-structure polycrystalline materials (< 10 µm) has been explained by GBS accommodated by slip. The experimental results on flow stress and strain rate dependence in fine-structure superplastic alloys are in conformance with the following relation [19]:

\[
\dot{\varepsilon} = A \left( \frac{h}{d} \right)^2 D_{GB} \left( \frac{\sigma}{G} \right)^2
\]

The stress exponent, n is 2. This is based on Gifkins [19] core and mantle model (Figure 2.10). In this model, grains are considered to be made of a separate core and mantle. The plastic flow consists of two independent processes: GBS accommodated by slip occurs in mantle region and slip occurs within the core of each grain. When the former dominates, superplasticity occurs.

Diffusion creep necessitates the grain-boundary sliding (GBS) in order to keep the grains in contact as the material is lost from longitudinal boundaries. Thus, to prevent the formation of voids or cracks during polycrystalline diffusional creep, additional mass-transfer must occur at grain boundaries. This result in GBS and the diffusional creep rate must be balanced exactly by the GBS rate if internal voids are not to form. Thus, GBS is an accommodating process to maintain the structural integrity. Diffusional flow and GBS are sequential process and both contribute to the total strain [12, 17]. Experimental investigations by Gifkins et al [20] have found that strain contribution by GBS is approximately 0.5 of the total strain. However, GBS does not contribute an independent strain and thus, its not easy to find its individual contribution to total strain. Stevens [16, 21] analyzed the grain boundary sliding occurring during diffusion creep theoretically and concluded that the grain geometry decides the relative velocities of displacement by GBS and by diffusion at a particular point on grain-
boundary. His formulation showed that GBS contribution to total strain is over 0.6 for materials with equiaxed grains of uniform size.

First mathematical framework to quantify the effect of grain-boundary sliding in high-temperature diffusion viscous flow of polycrystalline materials at low stresses was given by Lifshitz [22]. In this model, the grains keep their neighbors same throughout the deformation.

![Diagram](image1.png)

Figure 2.10: Gifkins [19] core and mantle model showing a mantle-like region within the region adjacent to the grain boundaries in Superplastic materials [4].

![Diagram](image2.png)

Figure 2.11: Diffusional deformation of an array of hexagonal grains. (a) Initial length $L$. (b) $L + \Delta L(d)$ after diffusional deformation. Dark regions represent separations. (c) $L + \Delta L(d) + \Delta L(s)$ after grain boundary sliding [24].
and is thus specific to diffusion creep. Rachinger [23] formulated a method for measuring the contribution of grain boundary sliding to axial strain by modeling the relative grain translations during plastic flow. Roger [24] later used Rachinger’s method to differentiate between Lifshitz sliding as “relative grain motion” and Rachinger sliding as “grain rearrangement” (Figure 2.11). Thus Rachinger sliding defines grain boundary sliding as a creep process in which grains exhibit no significant elongation but they become displaced with respect to each other so that there is a net increase in their number lying along the tensile axis. It occurs both under conditions of high temperature creep when the grain size is reasonably large and in superplasticity when the grain size is very small (< 10 µm) [12]. Lifshitz sliding, on other hand, is an accommodation phenomenon in diffusion creep at low stresses and low temperatures. Figure 2.12 shows the difference between Lifshitz sliding and Rachinger sliding.

![Figure 2.12: A uniform hexagonal grain structure under tensile stress. (a) Lifshitz sliding where grains keep same neighbors. (b) Rachinger sliding with grain rearrangement [26].](image)

A characteristic difference in grain-boundary sliding occurring in power-law creep and diffusion creep is that in former, it depends solely on the resolved shear stress on a particular boundary, while in latter, it depends on the difference in tensile stresses between various pairs
of boundaries. Thus sliding direction of one particular grain with respect to another will depend on the relative sliding between that grain and each of its neighbors.

2.3 Grain Boundary Diffusion

Grain Boundary (GB) diffusion plays a key role in many processes such as Coble creep, sintering, diffusion induced grain boundary migration (DIGM), recrystallization and grain growth. It controls the evolution of structure and properties of engineering materials at elevated temperatures. GB diffusion is not only important at elevated temperatures, but also at relatively low, even ambient temperatures. Grain boundaries have a typical thickness of a few atomic diameters, and thus they exhibit many properties of a two-dimensional system, which makes GB diffusion a physical phenomenon of great fundamental interest. Since a GB is a highly disordered two-dimensional plane between two highly ordered, but misaligned, single crystals, it is an ideal region for preferred transport of atoms. Thus, GBs provide high diffusivity paths, resulting in an accelerated atomic transport. GB diffusion characteristics are sensitive to the GB structure and chemical composition. They can be measured by modern radiotracer methods without disturbing the GB state. These GB Diffusion measurements are used as a tool to study the structure and properties of GBs [27, 28, 29].

2.3.1 Basic Model of Grain Boundary Diffusion

The most widely accepted model for GB diffusion is the Fisher model [30], which considers diffusion along a single GB normal to the surface. Most mathematical treatments are based on this model and propose solutions optimized by their own set of conditions. The GB is modeled by a high-diffusivity slab, of width $\delta$, embedded in a low-diffusivity bulk. Both the GB and bulk materials are assumed to be uniform and isotropic media which follow the Fick’s Law with the diffusion coefficient $D_b$ and $D$ respectively. This model is shown
schematically in Figure 2.13. The diffusing atoms initially deposited on the surface, penetrate fast along GB and are partly lost to the surrounding volume (grains). It is assumed that $D_b >> D$.

### 2.3.2 Mechanisms of Grain Boundary Diffusion

GB diffusion is a complex process and many studies have been conducted to further its understanding. Among these, atomistic simulations studies play a significant role. It has been established using these simulations that the ordered structure of GBs in metals can generate, absorb and support vacancies, which can move along the GB core by exchanging with individual atoms. Interstitials also play an important role in GB diffusion. Thus, GB diffusion can be described as a complex process involving different point defects, multiple jump processes, non-trivial jump-correlation effects, and other aspects [27, 28, 31]. The most favorable mechanisms of GB diffusion have been identified by Molecular Dynamic simulations. Vacancies typically move by exchanges with individual atoms. They can also make long jumps by exchanging with two or more atoms jumping simultaneously. Such long jumps are associated with vacancy instability during relaxation with neighboring atoms.
movements. These long jumps have activation energies comparable with those for single-atom jumps. Interstitial always move by collective jumps involving several atoms. Ring mechanism also operates in GBs. It can either be initiated by a point defect, or happen simultaneously in a defect-free GB. It involves several (upto 6) atoms jumping simultaneously. GB diffusion is much faster than lattice diffusion because GBs show a larger multiplicity of point defects and their migration mechanisms. Also, the defect formation energies and migration barriers in GBs are lower than those for lattice vacancies [29].

2.4 Diffusional Flow and Creep

Diffusional creep theory is based on the sound physical principle that the concentration of vacancies near a grain boundary is disturbed from the thermal equilibrium in the presence of a normal stress. Vacancy diffusion, driven by the concentration gradients resulting from an externally applied stress leads to the development of creep strain. Diffusional creep became focus of study and gained importance after the analysis of Coble [15] and Nabarro-Herring [13-14]. These theories could also predict appreciable rates reasonably accurately in polycrystalline materials under conditions that could be important technologically. The importance of grain-boundary sliding as an accommodation process to maintain the coherency in the material was pointed out and studies were done to find its contribution in the deformation by diffusional creep. Detailed examination of diffusion creep was first done by Lifshitz [22], who formulated the boundary conditions required to meet the coherency requirements.

Raj and Ashby [32] studied in detail the grain-boundary sliding with elastic and diffusional accommodation at arbitrarily shaped boundaries described by Fourier series, under shear stress. Under purely elastic accommodation, internal stresses grow as sliding proceeds until
they are balanced by the applied stress. This sliding is recoverable i.e. boundary slides back when the stress is released. The relative sliding displacements and normal stresses were accurately calculated. The applications of these equations to a sinusoidal shaped boundary, saw-toothed boundary, stepped boundary and a polycrystal resulted in a very small value of sliding.

Raj and Ashby tackled the diffusion creep problem by reducing it to diffusion accommodated sliding. Using this formalism, they calculated the sliding rate of a sinusoidally shaped boundary controlled by lattice and grain-boundary diffusion. The solution for sliding rate comes out to be linear and thus it can be applied to any arbitrarily shaped boundary using Fourier analysis. The diffusion rate was also calculated under a given shear stress using the sliding rate and considering a two-dimensional grain structure as a superimposition of two sets of zig-zag boundaries. Strain rate is given by:

$$\dot{\varepsilon} = 40 \frac{\sigma \Omega}{kT \Gamma^2} D_L \left( 1 + \frac{\pi \delta' D_{GB}}{\lambda D_L} \right)$$

The underlying principles of this approach are:

a) For steady-state deformation, the net flux of atoms into or out of each element of a boundary should precisely account for the normal component of the grain-boundary displacement.

b) The flux of atoms is provided by the lattice and boundary diffusion.

c) Normal stresses on a boundary drive diffusive flow at a rate that exactly compensates for the normal component of displacement at each point on the boundary.

The difference in the stress-distribution arising from grain-boundary sliding with elastic accommodation and that with diffusional accommodation at a saw-tooth boundary and
stepped boundary are shown in Figure 2.14. One can see that the stress profiles are very different for both grain boundaries under the two accommodation mechanisms.

Figure 2.14: Sliding at saw-toothed and stepped boundary showing elastic accommodation and diffusional accommodation [32].


2.5 Models for Creep Simulation

2.5.1 Ashby and Verrall “Grain-Switch” Model

This model was proposed by Ashby and Verrall [33]. They postulated that in grain-boundary sliding with diffusional accommodated flow, grain shape is preserved by a “grain-switching” mechanism that also produces a material strain. In order to maintain the matter continuity, grains remain stuck together and suffer a shape change by *accommodation strain*. These accommodation strains are accomplished by diffusion. This diffusion can be bulk-diffusion (Nabarro-Herring) or grain-boundary diffusion (Coble). The geometric representation of the model is given in Figure 2.15. In this geometry of two-dimensional configuration of four-grains, a true tensile strain of 0.55 is obtained as a result of grain-switching event.

The significant features of this switching mechanism are:

(a) The increase in the grain-boundary area as shown in Figure 2.14 (b) in the intermediate stage results in a ‘*threshold stress*’ below which switching is not possible.
possible. Thus, the applied stress must perform the work associated with the formation of increased grain-boundary area. Hence, the stress required for diffusional flow must be more than this threshold stress.

(b) Shape accommodation is provided by the diffusional flows as shown in Figure 2.16.

(c) Shear displacements occur in grain boundary plane (Figure 2.17).

Figure 2.16: Diffusional flow to effect the shape-change [33].

Figure 2.17: Sliding displacement and relative shear translations [33].
The strain rate equation for this model system is:

\[
\dot{\varepsilon} = \left( \frac{100\Omega}{kTd^2} \right) \left( \sigma - 0.72 \frac{\gamma}{d} \right) D_L \left( 1 + \frac{3.3\delta'D_{GB}}{dD_L} \right)
\]

where \(d\) is the grain diameter, \(D_{GB}\) is grain-boundary diffusivity, \(D_L\) is lattice diffusivity, \(\Omega\) is atomic volume, \(\delta'\) is the width of diffusion zone along grain-boundary and \(\gamma\) is the grain-boundary free energy. The term \(0.72 \gamma/d\) represents the ‘threshold stress’ for grain switching.

When only boundary transport is important, \(3.3\delta'D_{GB} \gg dD_L\), and Equation (14) reduces to

\[
\dot{\varepsilon} = \left( \frac{330\Omega}{kT} \right) \left( \frac{\delta'D_{GB}}{d^3} \right) \left( \sigma - 0.72 \frac{\gamma}{d} \right)
\]

The strain-rate as predicted by this model is approximately 7 times faster than that predicted by Nabarro’s (or Coble) diffusional creep. The main reasons for this are:

(a) The diffusive path lengths are shorter (by a factor of 3) in this model as compared to those in pure diffusional creep.

(b) There are 6 diffusive paths in this model as compared to only 4 in diffusion creep (Figure 2.18).

Figure 2.18: Comparison of (a) non-uniform diffusion accommodated flow and (b) quasi-uniform diffusional flow [33].
Ashby and Verrall model was supported experimentally by Naziri et al [34] on their work in Zn-Al eutectoid as shown in Figure 2.19. The grain-switch from Al-Al neighbors to Zn-Zn neighbors can be clearly observed. Further improvement in this approach was done by Ashby et al [35] using simplified bounding theorems for strain energy to perform approximate calculations for the strain rate in small-scale as well as large-scale diffusional flows. Using the principle of virtual work and strain energy they formulated the expressions for upper and lower bound for the strain-rate and concluded that rate of large-strain flow is faster than that at small strains because of the repeated grain-switching events.

Figure 2.19: Relative motion of zinc and aluminum grains during deformation of a Zn-Al 4 \( \mu \text{m} \) eutectoid foil at 100 °C [34].
2.5.2 Spingarn and Nix Model

Spingarn and Nix [36] analyzed the problem of diffusional creep and grain rearrangement by studying the normal tractions acting on a grain-boundary in a perfectly regular hexagonal structure. The assumptions of this model include: grains are elastically rigid, only diffusional relaxation is permitted during the flow and grain-boundaries are flat i.e. chemical potential of atoms on either side of the boundary is same to prevent grain-growth. This model provides an exact description of the equilibrium boundary traction distribution during steady state flow. This model discusses the stress distribution in terms of:

(a) the elastic response before any grain-boundary sliding or diffusion
(b) the stress state after grain boundary sliding but before diffusion
(c) steady-state stress distribution during diffusional creep.

The significant features of this model are:

(a) After initial loading, normal stresses on the boundary induce the chemical potential between grain boundaries leading to grain-boundary sliding with elastic accommodation. This results in change in traction distribution and boundary chemical potentials.

(b) Compressive tractions are introduced on grain boundaries near grain corners and tensile at the center of grain boundary segment. This helps to develop an initial transient diffusional flux until the potential gradient disappears. Thus, there is no diffusional flow from one end of grain-boundary segment to the other.

(c) Diffusional flow brings further changes in the traction distribution by inducing a flow of atoms from inclined grain boundary OX to the horizontal grain boundary OY as shown in Figure 2.20. Since the rate of deposition of atoms on OY is to be balanced
by rate of removal of atoms from OX and OX', hence, the steady state diffusion is
governed by relative speed (v) of separation of grains A and B.

Figure 2.20: Atomic motion in a hexagonal grain structure [36].

Figure 2.21: Distribution of the normal tractions along the grain boundary segments OX and
OY [36].
Thus, the basic principle of this model is that under steady state conditions, the flow of atoms to or from a boundary does not change the normal traction distribution thus maintaining elastically rigid grains and maintaining the grain continuity. The strain rate at the onset of deformation is found to be:

\[
\dot{\varepsilon} = 36 \left( \frac{D_{GB} \delta'}{d^3} \right) \left( \frac{\sigma \Omega}{kT} \right)
\]  

(16)

where \( \Omega \) is atomic volume, \( \delta' \) is the grain-boundary thickness and \( D_{GB} \) is the grain-boundary diffusivity. Using this approach, the normal tractions on a boundary segment can be calculated and are shown to vary from \( 2\sigma \) in tension to \( 0.25\sigma \) in compression (Figure 2.21).

It is worth mentioning that the Ashby-Verrall model [33] is limited to a system of only four grains and thus does not satisfy equilibrium conditions in large systems. Moreover, it is only valid to describe the behavior at large strains (> 0.55). At small strains (<0.5) and infinitesimal strains (< 0.01), it predicts lower strain rates than those defined by Nabarro-Herring-Coble equations. The Spingarn-Nix model gives an exact solution of the diffusional flow satisfying both compatibility (grain continuity) and equilibrium conditions (stress boundary conditions). Moreover, for single phase materials, this model predicts grain-switching by grain-boundary migration (Figure 2.22) as it does not support the diffusion paths of Ashby-Verrall model. This is because, Spingarn-Nix model does not allow the change in angle of grain-boundary segment with its neighbors.

In two-phase materials, this model induces boundary fluxes of same sign in both components by tractions across the phase boundary. Thus faster diffusing species can collect at a triple junction and cause grain neighbor switching by the wedging of two grains apart as shown in Figure 2.23. This is in experimental agreement with Naziri et al [34] (Figure 2.19).
Though the physics of the process and the solution is exact and appropriate for the systems discussed, this model is limited to only homogeneous structures.

Figure 2.22: Reaction paths for grain-switching (a)-(c) diffusion, (d)-(e) grain-boundary migration [36]

Figure 2.23: Two phase grain structure undergoing diffusional creep [36]
2.5.3 Hazzeldine and Schneibel Model

The earlier models have been derived considering a uniform microstructure with grains of same size. However, different grain shapes in one microstructure will result in a change in the lengths of diffusion paths, thus leading to different creep rates. Any real polycrystal consists of grains with different shapes and sizes. Different grain size distributions and grain arrangements will deform at different rates for same applied stress. Also, due to a strong inverse dependence on diffusion creep on grain size ($1/d^2$ or $1/d^3$), there will be higher stresses acting on larger grains. Schneibel et al [37] investigated various aspects of diffusion creep in microstructures with bimodal distribution of square grains in two dimensions and found that strain-rate increase by a factor of 4.4 and internal stresses as high as 3.5 times the applied stress can be found in some distributions. Following these results, Hazzeldine and Schneibel [38] proposed a formulation of the diffusion-accommodated sliding in irregularly shaped grain boundaries in a finite bicrystal. The assumptions of this model are: grains adjoining the boundaries are rigid, the boundaries do not support any shear stresses, sliding displacements are infinitesimal, rotation rate between the adjacent rigid crystals is infinitesimal and sliding is accommodated by only grain boundary diffusion.

This simulation model worked on the principle of dividing grain-boundary into small segments. In this model, for a grain boundary consisting of n straight segments, the stress distributions and sliding rates could be calculated by generating a system of 4n linear equations and then solving for the 4n constants, by implementing boundary conditions. The boundary conditions depend on the stresses or fluxes at the rigid endpoints of the grain boundary, matter continuity, rotation rates and plating rates along the boundary. The
numerical results obtained by this simulation model for a 35 segment sinusoidal grain boundary were in good agreement with the analytical results derived by Raj and Ashby [32].

The stress distribution along the boundary under the condition of no-flux at endpoints i.e. no surface diffusion results in very significant stress concentrations for a saw-tooth boundary (Figure 2.24) and a 45° inclined boundary with random bumps of different sizes (Figure 2.25).

Hazzledine and Schneibel have extended this methodology (breaking a grain boundary into n elements to calculate sliding distances and strain-rates) to predict the creep behavior in irregular, two-dimensional grain structures (25 grains) consisting of straight grain boundary segments connected by triple points [39]. The results for a regular hexagonal structure were in

![Figure 2.24: (a) Saw-tooth boundary subject to a pure shear stress. (b) Stress-distribution for no-flux condition at end points [38].](image1)

![Figure 2.25: (a) 45° inclined boundary with equidistant bumps of random sizes. (b) Stress-distribution for no-flux condition at end points [38].](image2)
complete agreement with the analytical derivations of Spingarn and Nix [33]. Figure 2.26 shows the initial grain structure under uniaxial loading, and its deformed structure as well as the distribution of normal stresses along a particular path. For an irregular structure, containing one large grain in the center, Hazzeldine and Schneibel’ simulations showed significant grain rotations, plating towards the corners and inhibition of necking by the large grain. The maximum stress reaches as high as $3.64 \sigma_a$ at corners.

This model was one of the first attempts to quantify the effect of grain size distribution and grain shape on the creep rate focusing on irregular structures. Since the formulation of this model does not involve any approximations, the corresponding simulation results are in perfect agreement with analytical models obtained earlier. However, this model is very difficult to implement for larger structures as it is based totally on the number of equations which in turn, are 4 times the total number of grain-boundary segments. Thus a better approach was still required to simulate larger systems closer to real microstructures.

Figure 2.26: (a) Regular hexagonal structure and (b) irregular structure with stress distribution [38].
2.5.4 Pan and Cocks Model

Cocks [41] applied finite-element analysis to the grain boundary diffusion process based on the variational principle formulated by Needleman and Rice [40]. Under this formulation, the length of a grain boundary is divided into a number of elements and degrees of freedom are associated with the translation and rotation of grains, the flux of vacancies across the center line of the boundary and the chemical potential at grain-boundary nodes. Cocks [41] produced exact results of the stress distribution in a regular hexagonal structure and the relative velocities experienced at the center of each grain. Moreover, in this formulation he considered the situation where both deformation and void growth results from diffusional transport of atoms along the grain boundaries.

Later, Pan and Cocks [42] used this numerical technique to solve the governing equations of grain boundary diffusion during superplastic deformation. This is, in principle, similar to a material under mechanical loading deforming by grain-boundary sliding accommodated by grain-boundary diffusion. The systems studied included a regular array of hexagonal grains and an irregular grain structure taken directly from a material micrograph (with straightened boundaries). This helps to understand the effect of randomness of grain size and shape on strain rate and deformation. The assumptions of this model are:

(a) Deformation results from diffusive flux of atoms along the grain boundaries.

(b) Grains remain rigid throughout the deformation.

(c) There is no resistance to relative sliding along the grain-boundaries i.e. grains do not support shear stress.

(d) There are no voids at grain-boundary junctions or cracks in the microstructure and matter is continuous.
The significant features of this computer simulation model are:

(a) The whole microstructure is first defined by dividing the grain-boundaries into small segments to which the corresponding degrees of freedom are associated.

(b) Tensile stress is then applied on the boundaries of the simulation box and the relative velocities of grain-centers are calculated using finite-element methodology based on the variational formulation for dissipated power.

(c) The grain boundary network is then updated according to the relative grain velocities after each time-step.

(d) Time step is defined by the strain increment thus affecting the rate of loading.

(e) Any four-rayed grain boundary junction is unstable and will result in grain-switch as shown in Figure 2.27.

(f) Vanishing grain boundaries lead to dynamic grain growth as shown in Figure 2.28.

![Figure 2.27](image1.png): Grain-Switch event by a vanishing grain boundary [42].

![Figure 2.28](image2.png): Vanishing grain boundary leading to dynamic grain growth [42].
The grain structure evolution for a regular array of hexagonal grains is shown in Figure 2.29 and for an irregular structure is shown in Figure 2.30. The results obtained for regular structure were similar to the Spingarn-Nix [36] analytical solution, thus proving the accuracy of the solution and the physical description of the process as well.

Figure 2.29: Grain structure evolution of a uniform array of hexagonal grains [42].

Figure 2.30: Grain structure evolution of an irregular microstructure [42]. One of the shaded grain shrank due stress induced grain growth.
Thus, Pan and Cocks model was the first model to provide exact solutions for strain-rate and stress distributions for regular and irregular grain structures. The computational technique using the iterative process is relatively convenient to implement for larger structures subject to the constraint of computational power. This principle has been successfully used to study similar systems such as void growth by grain-boundary diffusion in fine grained materials where void spacing is more than the grain size, which in turn is more than the void radius [43], void growth ahead of a dominant crack in a material deforming by grain-boundary diffusion [44], coupled surface and grain-boundary diffusion [45] and grain-boundary migration as well [46]. Various other models like dislocation climb at grain boundaries using slip-band model by Spingarg-Nix [47], interface controlled diffusion creep governed by non-conservative motion of boundary dislocations [48], Gifkins [49] grain-emergence model (emergence of a grain from layer beneath after fissuring of sliding grains) have been proposed to investigate the sliding accommodated diffusion. But in all of these models the detailed physical process is not described and they simply postulate topological grain rearrangements during structure evolution. These models mainly try to explain the structure evolution in terms of the characteristic feature of the superplastic deformation/diffusion creep i.e. grains preserve their shape very till large strains. Moreover, all these models can only deal with ideal regular grain structure. However, in Pan and Cocks model not only the approximately equiaxed grain shapes are retained to large strains, but it also features grain rotations and grain-vanishing due to stress-induced grain growth. Thus, it can be said that this model not only explains the physical phenomenon, but also the microstructural features and can be successfully applied to study more realistic microstructures than just purely regular ones.
3. Problem Formulation

As mentioned earlier, diffusion creep is significantly affected by the grain size and shape, owing to its inverse dependence on $d^2$ and $d^3$ for bulk diffusion and grain-boundary diffusion respectively. Presence of microstructural inhomogeneity, thus, not only affects the strain rate during diffusion creep, but it also changes the stress-distribution in the system giving rise to stress concentrations at grain boundaries. These stress concentrations play a critical role in nucleation of cavities and crack nucleation along grain-boundaries. Most of the earlier studies in this area have been performed on small idealized grain structures [33, 36] and only a very few have been focused on small irregular structures [39, 42], and that too, containing one small inhomogeneity only. These studies can satisfactorily provide a general view of the phenomenon, but in order to get a deep insight of the physical process, we have to study larger systems containing multiple inhomogeneities. These studies would help us to find out the interactions within the inhomogeneities in terms of stress-distribution and the long-range stress relaxations in the structures. Experimental investigations help in characterizing the strain rates into various regimes by analyzing the microstructures, but they do not provide any method to measure stress concentrations at internal interfaces.

Computer simulations come here as a handy tool to investigate these stress concentrations by focusing on the physics behind the process. Complex mathematical formulations can be solved using pertinent algorithms and computational power. Moldovan et al [50] have studied the stress concentrations along grain boundaries in perfectly regular hexagonal structures and grain structures containing one large grain at the center. Microstructural inhomogeneity in the form of large grain was 2.3 and 4.2 times larger than the regular hexagonal grain. Figure 3.1 shows a regular homogeneous microstructure containing 150 grains subjected to externally
applied stress $\sigma_o$. It can be observed that the normal stresses vary from $2\sigma_o$ to $-0.25 \sigma_o$. The stress distribution is uniform for this structure.

Figure 3.1: A regular hexagonal grain structure subjected to uniaxial tensile stress $\sigma_o$ and the stress distribution along the selected grain boundary path [50].
Figure 3.2: Topologically inhomogeneous grain structures consisting of regular hexagonal structure with a larger grain in the middle. (a) 2.3 times and (c) 4.2 times that of a regular hexagonal grain. (b) and (d) represent the stress concentrations along selected GB paths [50].

Significant change in the stress concentrations from the one in Figure 3.1 can be observed in Figure 3.2 for microstructures consisting of one larger grain at the center. Not only the tensile stresses but compressive stresses are also significantly altered. Thus, it can be seen that even small inhomogeneity can have significant effect on the stress distributions. In this study we will focus on different microstructural topologies consisting of one and more than one large grain of various sizes in different arrangements in a regular structure.
4. Simulation Methodology

4.1 Mesoscopic Simulation Approach

The mesoscopic scale refers to the length scale at which one can reasonably discuss the properties of a material or phenomenon without having to discuss the behavior of individual atoms. For practical purposes, the mesoscopic scale is the size at which it becomes reasonable to talk about the average density, charge or other characteristics of a material, and where statistical properties such as temperature and entropy have meaning. Since, dealing with individual atoms is mathematically complex, calculations are often performed by averaging over structure "at the mesoscopic scale", thus replacing the discrete structure of atoms with a continuous distribution of mass, charge, etc, whose values are taken as equal to that from averaging over several thousands atoms in that vicinity. For many problems, such mesoscopic averaging allows one to very accurately predict macroscopic behavior and properties. The mesoscopic scale thus lies between the macroscopic scale of the world we live in, and the atomic scale in which each atom is considered separated resolved. For technical purposes, the mesoscopic scale is the size at which the expected fluctuations of the averaged properties due to the motion and behavior of individual particles can be reduced to below some desirable threshold (often a few percent), and must be rigorously established within the context of any particular problem.

Mesoscopic simulations represent an important layer of information between the atomistic and macroscopic descriptions of mechanical behavior. Such simulations involve a much reduced number of variables compared to atomistic ones, thus allowing the modeling of the microstructure evolution over much longer time and length scales, and helping to formulate constitutive relations to be incorporated into macroscopic models. The mesoscopic simulation
is less detailed in its output than is microscopic simulation, but it is more computationally efficient, thus, making it possible to solve large-scale microstructures.

### 4.2 Simulation Model

In this study, the microstructure of a 2D polycrystal is represented by a hexagonal grain system consisting of grain boundaries and symmetric three-fold nodes. The theoretical approach for investigating the microstructural evolution in our mesoscopic simulation study is based on the variational principle for dissipative systems, originally formulated by Needleman and Rice [51] for grain-boundary and surface diffusion in context of grain growth.

This study is based on the approach of Pan and Cocks [42] and Cocks and Searle [43]. The equations and the concepts used in our mesoscopic simulation are explained below (For more details, see Appendix A). The diffusion of atoms along grain boundaries is driven by the gradient of the chemical potential, which is induced by the gradient of the stress, \( \sigma \), acting along each boundary. The chemical potential in the GB plane is related to the stress, \( \sigma \), by the relation:

\[
\mu = \mu_0 - \sigma \Omega \tag{17}
\]

where, \( \mu_0 \) is the chemical potential of an atom in a stress-free system and \( \Omega \) is the atomic volume. From Fick's first law, the diffusive flux along each GB can be shown to depend on the gradient of the normal-stress component, \( \sigma_n \), along the GB as follows:

\[
J = \frac{D_{GB} \delta \Omega}{kT} \frac{\partial \sigma_n}{\partial s} . \tag{18}
\]

Here \( s \) is the local spatial coordinate along the diffusion path, \( D_{GB} \) is the grain boundary self-diffusion coefficient, \( \delta \) is the diffusion width of the grain boundary, \( k \) is the Boltzmann's constant and \( T \) is the absolute temperature. The atoms diffusing along the grain boundaries
can be either deposited at the grain boundaries or removed from them. These processes cause grains on either side of the boundary to move with respect to each other in a direction normal to the GB at a rate $v_n$. Conservation of matter requires that

$$\frac{\partial J}{\partial s} + v_n = 0 \quad .$$

(19)

Using Equation (17), $v_n$ can be calculated as:

$$v_n = -\frac{D_{GB} \partial^2 \sigma_n}{kT \partial^2 \delta} \quad .$$

(20)

Assuming also that no microcracks or voids are allowed to open up at the grain boundaries or triple junctions, thus allowing continuity of matter, the fluxes $J_i$ along the three grain boundaries meeting at a triple junction must satisfy the condition

$$\sum_{i=1}^{3} J_i = 0 \quad .$$

(21)

where, $J_i$ is considered positive for the fluxes flowing into and negative for those flowing out of the triple junction. Equations (17)-(21), together with specified border conditions imposed on the simulation cell, describe the deformation process of a polycrystal with any grain topology and may be implemented in a computational framework. This computational implementation follows the approach described by Cocks [42] and is based on the Needleman and Rice [51] variational functional. Cocks demonstrated that the solution is given by the velocity field, \{\$v_n\}, and flux field, \{\$J\}, along each GB in the system. These fields minimize the functional

$$\Pi = \int_s \frac{kT}{2D_{GB} \partial^2 \delta} J^2 ds - \int_{\Gamma} T_{ij} V_{ij} d\Gamma \quad ,$$

(22)
subjected to the constraint of equation (21). Here $S$ is the total length of the grain boundaries through which the diffusional flow takes place, $\Gamma$ is the length of the border of the simulation cell moving with velocity $V_i$ when an external stress, $\sigma_o$, is applied. $T_i = \sigma_o \Gamma_i$ is the value of the traction exerted on the segment of length $\Gamma_i$ located on the simulation-cell border (see Appendix B).

The contribution to equation (22) from each GB segment can be written explicitly in terms of the following local degrees of freedom [43]: the velocity components of the center of mass of the two grains determining the GB, the rates of rotation of the grains, the value of the diffusional flux in the middle of the GB segment and the values of the normal stresses at the ends of the GB segment. The numerical method used here to minimize the variational functional follows the standard finite-element procedure [42] (refer to Appendix C and D). The schematic representation of this process is shown in Figure 4.1.

![Figure 4.1](image)

Figure 4.1: A schematic representation of diffusion flow creep, when $J_a > J_b$ (incoming flux is more than outgoing flux) and grain-boundary thickness $\delta$, increases by relative velocity, $v_n$.

This leads to the following matrix equation:

$$[G][U] = [F]$$  \hspace{1cm} (23)

where, $[G]$ is the generalized stiffness matrix governed by the material properties, conservation law and simulation-border conditions. $[U]$ is the global column vector of degrees
of freedom and \([F]\) is the external force vector which contains information on the external forces applied along the border of the simulation cell (Appendix E). The solutions of equation (23) are obtained by using a linear solver. For details about the updating of microstructure during deformation and node attraction, refer to Appendix F and G.

### 4.3 Initial Microstructures with Inhomogeneities

The initial microstructures are generated by using mesoscopic simulations of anisotropic grain-growth. It consists of interconnected polygons, initially generated by a Voronoi construction, with periodic border conditions applied to the simulation cell. Each grain is assigned an initial orientation with respect to a fixed axis in the plane of simulation cell, thus characterizing each grain-boundary by the misorientation angle between two neighboring grains. It is assumed that during grain-growth, this orientation does not change [52]. In order

![Initial microstructures](image)

Figure 4.2: Initial microstructure with 480 grains and one biased grain at center subjected to abnormal grain growth.
to achieve abnormal grain-growth i.e. selected grain (or grains) grow more than other, the selective grain (or grains) are biased by modifying their grain-boundary energy and mobility simultaneously. The selected grain (or grains) grows abnormally, generating inhomogeneous microstructures with varying size of inhomogeneity.

From the various microstructures generated, a few are selected on the basis of the size ratio of the abnormal grain and normal hexagonal grain. These selected microstructures are then converted from periodic border to finite border, thus, enabling them to be used for creep deformation. This conversion increases the number of grains, as it counts the half-cells at the boundaries and introduces a finite boundary on the simulation cell. This is imperative, as the simulations for creep assume mass-conservation and no diffusive flow at the external simulation cell boundaries.

![Microstructure](image)

(a) 426 grains  
(b) 459 grains

Figure 4.3: A microstructure with 426 grains under periodic border conditions has 459 grains when converted to finite border condition.

### 4.4 Topological Changes in Microstructure

During grain growth the average grain diameter and grain area increases. This happens as some grains grow while others shrink and eventually disappear. Thus, the topology of the system evolves continuously. Similarly, during creep deformation certain vertices come closer...
to each other as matter diffuses out of the grain-boundary connecting those two vertices. Therefore appropriate actions must be incorporated into the simulation algorithm to account for possible discrete topological changes. In one of the first simulation studies on time evolution of cells structures, Weaire and Kermode [53] have defined three such basic topological transformations. One can also show that the whole range of topological changes occurring in an evolving microstructure can be obtained from a finite combination of the following discrete topological events:

4.4.1. T1 Switch

T1 switch represents the neighbor-switching event, which occurs when a grain boundary becomes shorter than some fraction $\Delta_{T1}$ of the scaled characteristic length in the system. In this study, the value of $\Delta_{T1}$ is taken as 2% of the scaled characteristic length. The schematic representation of a T1 switch is shown in Figure 4.4. Nodes C and D come closer to each other and the grain boundary length ($\Delta$) falls within the critical length defined in the simulation. Prior to T1 switch grains A and B were the neighbors. After T1 switch, grains C

![Figure 4.4: Schematic representation of T1 neighbor switching event.](image)

![Figure 4.5: Schematic representation of a T2 switching event.](image)
and D become neighbors with a slight increase in the grain boundary length \( [\Delta(l+\varepsilon)] \) between nodes A and B. The transformation can be visualized as a continuous process with an intermediate state represented by the middle figure, which is physically unstable.

4.4.2. T2 Switch

T2 switch is a three-sided cell disappearance event, which occurs when the area of a grain becomes smaller than some fraction \( \Delta_{T2} \) of the scaled characteristic area (0.1 %) in the system. The grain is observed to be three-sided and is removed from the network during the switch. In Figure 4.5, the area of grain A becomes smaller than the scaled characteristic area in the system. Thus, it is removed and a new triple junction is created with grains B, C and D.

4.4.3. T3 Switch

T3 switch is a two-sided cell disappearance event, which takes place when a two-sided cell consisting of only two triple junctions is formed due to a T1 or T2 switch. Figure 4.6 shows how a T2 switch generates a two-sided grain. A T3 switch is followed restoring a stable microstructure.

Figure 4.6: Schematic representation of T3 switching event.
5. Results and Discussion

5.1 Effect of Inhomogeneity on Stress Distribution in the System

Presence of inhomogeneities in the microstructure has a significant affect on the mechanical properties of a polycrystalline material. Inhomogeneities result in stress concentrations at grain boundaries, an important phenomenon bearing a direct consequence on crack nucleation and creep fracture at elevated temperatures. Fracture is essentially a process of rupture of atomic bonds across localized regions of material resulting from the growth of an imperfection or flaw under an applied external force. Although, conceptually a simple physical process, the selection of sites for nucleation of cavities or crack along a grain-boundary or for dislocation emission from a grain-boundary is critically related to the stress concentrations at the grain boundaries. At low temperatures, stresses are larger at triple junctions and deformation is governed mainly by dislocation activity. However, at elevated temperatures, when diffusion creep is the dominating process of deformation, these stress concentrations are located at the center of the grain boundaries. Generally, larger grains act as the sources of stress concentrations [50, 54].

In the present study, the focus is to study the effect of various inhomogeneities on the stress distribution in the microstructure subjected to uniaxial tensile stress. Inhomogeneities are described in the form of a single grain of varying sizes and also in the form of two, three and four grain clusters. The total area of inhomogeneity is kept constant at approximately about 15% of the total microstructure area. Stresses are determined along selected grain-boundary paths which are crossing the structure perpendicular or parallel to straining direction. The results are then quantified in terms of size-ratio (i.e. area of inhomogeneity to area of a regular hexagonal grain i.e. $A_{\text{Inhom}}/A_{\text{Hex}}$).
5.1.1 Microstructures with Single Large Grain

In Figure 5.1, there are approximately 429 regular grains, 30 smaller four or five-sided grains and one equiaxed large grain at center with area 66.5 times that of regular hexagonal grain. It accounts for about 13.5% of the total area of the simulation system. Comparing the five stress distributions it can be observed that: i) the amplitudes of the stress distributions along the median paths A, B and E, that intersect the larger grain are larger than the amplitudes along the paths C and D (those that do not touch the larger grain) ii) the
compressive stresses along paths C and D are significantly smaller and act on significantly fewer grain boundaries than along the paths A, B and E iii) the normal stress distributions converge to the characteristic periodic distribution of the normal stress in a uniform regular structure under stress [50] (characterized by a maximum stress that is twice the value of the externally applied stress, $\sigma_0$) faster along the paths A, B and E than along paths C and D and iv) the maximum normal stress in the microstructure, $\sigma_n = 3.25 \sigma_0$, is found along path C at the center of a GB located about one grain diameter away from the surface of the large grain. This can be explained by the fact presence of smaller grains (smaller than the hexagonal matrix grains) surrounding the large central grain, which contribute directly to lowering the stress concentration on the surface of the larger grain. This similar fact can be observed in path E, with the maximum normal stress peak on the both sides of the larger grain.

Figure 5.2 shows a microstructure with 470 regular grains and one large grain surrounded by 12 smaller grains. The larger grain is 34.3 times the area of regular grain accounting for 7.2% of the total simulation cell. Apart from the observations similar to earlier system, it can be seen that maximum normal stress, $\sigma_n = 3.36 \sigma_0$ is along path B, topologically similar to the previous structure but higher value. Although the size of smaller grain is approximately same in both these systems, the smaller size of large-grain in this system contributes to a higher value. Normal stress distribution converges to the one corresponding to a regular structure along path D, showing stress relaxation as we move apart from the inhomogeneity. Similarly, comparing paths E in Figure 5.1 and Figure 5.2, we can observe a higher value of stress factor attaining the normalized value fast in Figure 5.2.
Figure 5.2: Microstructure with 483 grains total and one large grain in center with $A_{\text{Inhom}}/A_{\text{Hex}} = 34.3$ and corresponding stress concentrations on the selected GB paths.

Figure 5.3 shows a microstructure with 475 regular grains and one large grain surrounded by 18 smaller grains. The larger grain is 25.4 times the area of regular grain accounting for 5.2% of the total simulation cell. This is equivalent to the one large grain of a three-grain cluster accounting for 15% of total area. Apart from the observations similar to earlier systems, it can be seen that maximum normal stress, $\sigma_n = 3.60 \sigma_0$ is along path B, topologically similar to the previous structures but a significantly higher value. Unlike earlier microstructures, no small grain is present in this system near the larger grain. Hence the contribution to this stress concentration is solely because of the inhomogeneity in the system.
Also it can be seen that the stress concentration rises as the size of inhomogeneity is decreasing. Comparing path C in Figure 5.2 and 5.3, which are topologically similar i.e. about 2 grain diameters away from the inhomogeneity, it can be seen that tensile stresses converge to the normal distribution slowly in Figure 5.2 than in Figure 5.3. This can be attributed to the presence of the small grain, which affects the stresses not only on the boundaries immediate to it, but also the ones in the surrounding region. Observation can be made about paths B of both the figures, by the absence of surrounding peaks in Figure 5.2.

![Microstructure diagram](image)

Figure 5.3: Microstructure with 495 grains total and one large grain in center with \( A_{\text{inhom}}/A_{\text{Hex}} = 25.4 \) and corresponding stress concentrations on the selected GB paths.
Figure 5.4: Microstructure with 501 grains total and one large grain in center with $A_{\text{Inhom}}/A_{\text{Hex}} = 17.6$ and corresponding stress concentrations on the selected GB paths.

Figure 5.4 shows a microstructure with 495 regular grains and one large grain surrounded by 6 smaller grains. The larger grain is 17.6 times the area of the regular grain accounting for 3.2% of the total simulation cell area. Maximum normal stress, $\sigma_n = 3.22 \sigma_0$ is along path B, which again can be attributed to the presence of a small grain. However, this value is overall lowered as the inhomogeneity is hexagonal and not circular.
5.1.2 Microstructure with a Two-Grain Cluster

Figure 5.5: Microstructure with 453 grains total and a two-grain cluster in center with $A_{\text{Inhom}}/A_{\text{Hex}} = 34.3$ & corresponding stress concentrations on the selected GB paths.

Figure 5.5 shows the microstructure in the presence of two larger grains located close to the center of the system. Each of the two larger grains has an area of about 34.3 $A_{\text{hex}}$, and their combined area is about 15% of the total system area. Similar to the system presented in Figure 5.1, the amplitude of the normal stress is larger along the median path A. Moreover for this system the maximum normal stress ($3.07 \sigma_0$) located along a GB on path B is only slightly larger than the stress ($2.89 \sigma_0$) at the tip of one of the larger grains (path A) and it is smaller
than the maximum stress (3.36 $\sigma_0$) found in Figure 5.2. Since, the system in Figure 5.2 represents a similar system with one inhomogeneity, it can be said that the presence of the cluster here has relaxed the stress concentrations. The effect of this stress relaxation is more pronounced as we move away from the center. This is evident from Figure 5.6, where the cluster is close to the bottom and the GB paths C and D are quite far away from it, close to the top. It can be noticed that along path D (about 9 grain diameters away from cluster), the normal stress distributions almost converge to the characteristic periodic distribution of the normal stress in a uniform regular structure. Thus, the effect of the change in diffusion paths along the cluster is not so pronounced as we move farther away from it.

Figure 5.6: Microstructure with 453 grains total and a two-grain cluster at bottom with $A_{\text{Inhom}}/A_{\text{Hex}} = 34.3$ & corresponding stress concentrations on the selected GB paths.
5.1.3 Microstructure With a Three-Grain Cluster

Figure 5.7 shows a microstructure with a three-grain triangular cluster located at the center of the system. Each of the three larger grains has an area of about 25.4 $A_{\text{hex}}$, and their combined area is about 15% of the total system area. This system is asymmetric and has the characteristics of the single-grain and two-grain cluster systems. The tensile stresses along path A are higher at the center (2.7-2.8 $\sigma_0$) rather than at the interfaces of the GB path and the larger grains (2.54 $\sigma_0$). This is because of the stress-raising effect of the third single grain. The largest normal stress $\sigma_n = 3.75 \sigma_0$ is located at the center of the GB path E, situated one
grain away from the surface of the large grain sitting at the tip of the triangular cluster. Comparing this result with the GB path B of Figure 5.3, which represents a single grain of same size, it can be seen that maximum normal stresses has increased. This is because of the effect of two-grain cluster at the bottom. Along GB path F, stress normalization is very fast around the two sides of the peaks. Comparing paths C and D, one can easily notice that stresses are higher along path D rather than C, even though they are along same grain. Similar observation can be made while comparing paths B and E. Thus, it can be concluded that this three-grain cluster act as a very prominent stress raiser, giving rise to stresses as high as 3.75 times the applied stresses at the tip. Such locations aid in crack nucleation and subsequent fracture. Also, higher stresses are found in the region above the tip of the cluster and stresses are relaxed in the lower half of the structure because of the symmetry induced by the two-grain cluster.

5.1.4 Microstructures with Four-Grain Cluster

Figure 5.8 shows a microstructure with a four-grain cluster located at the center of the system. Each of the four larger grains has an area of about 17.6 Å\textsubscript{hex}, and their combined area is about 15\% of the total system area. There are 24 smaller grains, i.e. 6 smaller grains surrounding each larger grain. This system is symmetric and stress distribution is also symmetric on the either side of the structure. The maximum value of tensile stress in this system is attained along the GB path B and it approaches 3.18 times the applied stress \(\sigma_0\). This is about 2 grain diameter away from the bottom large grains and one grain diameter away from top large grains. Presence of a small grain close to the larger grains also contributes in this stress concentration. However, this stress is significantly higher than the maximum stress achieved along the paths A and C which are along the larger grains.
Figure 5.8: Microstructure with 465 grains total and a four-grain cluster in the center with $A_{\text{Inhom}}/A_{\text{Hex}} = 17.6$ & corresponding stress concentrations on the selected GB paths.

Maximum tensile stress along the path D which is on the small grain (surrounding the larger grain) is $2.9 \sigma_0$. This is lower than that along path B. Also, along path A and C, which are similar, but topologically different, one can notice that tensile stresses are higher along A, which goes through inside the cluster, rather than C, which goes through the outer side. Thus, it can be concluded, that in this cluster, though stresses are relaxed as compared to those in a three-grain cluster, but still stress-distribution is uneven and stresses are higher in the regions inside the cluster than those on the outer sides.
Figure 5.9 shows a similar microstructure with a diamond shaped four-grain cluster located at the center of the system. This system is also very symmetric and stresses are relaxed. Maximum value of tensile stress is along path B in the middle of the structure and it reaches about 3.1 $\sigma_0$. This region is again located inside the cluster. Interestingly, stresses along the path C are not very significantly high, even though it is one grain away from the larger grain and is located inside the cluster. Rather the maximum stress along this path is 3.05 $\sigma_0$, which is same the maximum stress along the path D.

Figure 5.9: Microstructure with 465 grains total and a diamond shaped four-grain cluster with $A_{\text{Inhom}}/A_{\text{Hex}} = 17.6$ & corresponding stress concentrations on the selected GB paths.
5.2 Effect of Inhomogeneity on Strain-Rate

In a simulation study, it is imperative to verify the accuracy of the algorithm by studying the already reported results or studies. The current study is based on the Pan and Cocks [42] model for coble creep deformation. The simulation methodology and the numerical technique, as explained earlier were first implemented to simulate the evolution of a regular array of hexagonal grains, subjected to a constant uniaxial stress. The structural evolution of a microstructure containing 513 uniform hexagonal grains at various levels of strain is shown in Figure 5.10. The normalized strain-rate as a function of strain (in %) is shown in Figure 5.11.

The results of our simulation are in perfect agreement with the simulation results of Pan and Cocks [42] and the Spingarn-Nix [36] analytical solution as well. From the structural evolution in Figure 5.10, it can be observed that the grain boundaries perpendicular to the stress direction shorten with the increasing strain and the 60º boundaries elongate. Since, boundaries can slide freely without any resistance, the stresses along these inclined boundaries do not change and the remaining perpendicular boundaries have to support same force over a decreasing area. This results in higher stresses along these perpendicular boundaries and thus a faster creep rate. This structure evolution goes on till 60 % of the strain is reached, when; all the perpendicular boundaries reach their critical length for the T1 switch. As strain further increases, symmetry of the structure is destroyed and the grain boundaries are able to rotate and slide past each other, leading to an equiaxed microstructure.

These results indicate that the current model is accurate and suitable for further studies. Results obtained for the inhomogeneous microstructures are classified as one-grain, two-grain and three-grain systems.
Figure 5.10: Grain structure evolution of a uniform hexagonal array.

Figure 5.11: Strain rate (normalized units) versus strain for the homogeneous microstructure.
5.2.1 Strain Rate for Microstructures with One Large Grain

The creep deformation in the presence of a single large grain in an otherwise uniform hexagonal microstructure was investigated for several different microstructures. Various inhomogeneous microstructures were quantified on the basis of the area ratio: $A_{\text{Inhom}}/A_{\text{Hex}}$, where $A_{\text{Inhom}}$ is the area of the larger grain/inhomogeneity and $A_{\text{Hex}}$ is the area of the regular hexagonal grain.

Figure 5.12: Snapshots showing the structural evolution during the creep deformation of a 507 grains microstructure with one large grain at center and $A_{\text{Inhom}}/A_{\text{Hex}} = 10.0$. 

\begin{itemize}
  \item $\varepsilon = 0\%$
  \item $\varepsilon = 20\%$
  \item $\varepsilon = 40\%$
  \item $\varepsilon = 50\%$
  \item $\varepsilon = 60\%$
  \item $\varepsilon = 65\%$
  \item $\varepsilon = 70\%$
\end{itemize}
Figure 5.12 shows the grain structure evolution during the creep deformation simulation of a microstructure with 507 grains and $A_{\text{Inhom}}/A_{\text{Hex}} = 10.0$. Upon close observation of the structure at 40% strain, grain boundaries parallel to the applied stress direction can be seen close to the inhomogeneity. This implies that grain-switching initiates as early as 40% of the strain. Similarly, grain-switch in different regions of the microstructure can be observed in subsequent snapshots at strains of 50, 60 & 70% respectively. An interesting fact to observe here is that most of the grain-switching events occur in the region exactly above and below the inhomogeneity. Moving diagonally from the inhomogeneity towards any of the corner vertex of the simulation cell, perpendicular boundaries can still be observed at strains as high as 70%. This implies that preferred diffusion paths are diagonal and the creep rate at higher strains is mainly due to diffusion along these boundaries.

Figure 5.13 shows the normalized strain rates for five such non-uniform microstructures plotted against the strain rate for the regular homogeneous microstructure [42]. The area of one large grain, $A_{\text{Inhom}}$ in the non-uniform microstructure is: 2.0, 4.0, 6.0, 12.1 and 27.8 times larger than the area of a hexagonal grain $A_{\text{Hex}}$. It is evident from Figure 5.12 that the presence of the inhomogeneity removes the singularity in the strain rate and the peak value of the strain rate has amplitude that depends on the area of the inhomogeneity. The larger the relative area $A_{\text{Inhom}}/A_{\text{Hex}}$ of the inhomogeneity, the smaller the peak value in the strain rate. Moreover, the peak position is also shifted towards lower values of the strain. Smaller peak values can be explained by the fact that the grain-switching events do not occur simultaneously like they do in a perfectly regular structure. Inhomogeneity induces the asymmetry in the structure and thus grain-switches at different boundaries occur at different times.
5.2.2 Strain Rate for Microstructures with Two Large Grains

Similar studies on creep deformation were carried out on different microstructures containing two large grains in an otherwise uniform hexagonal microstructure. Figure 5.14 shows the microstructural evolution during the creep deformation simulation of a microstructure containing total of 501 grains and two large grains with $A_{\text{Inhom}}/A_{\text{Hex}} = 10.0$. Similar observations could be made here like the ones in Figure 5.12. Grain-switching events can be observed in the vicinity of both the larger grains at lower strains of 40 % and the perpendicular boundaries can be seen along the diagonal paths surrounding the larger grains. However, in this case, these preferential diffusion paths do not extend till the corners of the simulation cell. This implies that the boundaries will be able to support lower stresses resulting in a low strain rate.

Figure 5.15 shows the normalized strain rates for five such non-uniform microstructures plotted against the strain rate for the regular homogeneous microstructure [42]. The area of
one large grain, $A_{Inhom}$ in the non-uniform microstructure is: 2.0, 4.0, 6.0, 12.1 and 27.2 times larger than the area of a hexagonal grain $A_{Hex}$. Similar to Figure 5.13, it can be seen here that the peak values of strain rate are lowered significantly and the peak shifts to the left to lower strains. Apart from this, flattening in the peak can also be observed with the increase in the $A_{Inhom}/A_{Hex}$ ratio. At a high ratio of 27.2, strain-rate curve is almost flat and attains peak value at very low level of strains implying continuous switching events.

![Figure 5.14: Snapshots showing the structural evolution during the creep deformation of a 501 grains microstructure with two large grains at center and $A_{Inhom}/A_{Hex} = 10.0.$](image)

Figure 5.14: Snapshots showing the structural evolution during the creep deformation of a 501 grains microstructure with two large grains at center and $A_{Inhom}/A_{Hex} = 10.0.$
Figure 5.15: Normalized stain rate vs. strain for the five non-uniform microstructures containing two inhomogeneities, plotted against the strain rate for homogeneous structure.

5.2.3 Strain Rate for Microstructures with Three Large Grains

Using similar approach, creep simulations were done on different microstructures containing three large grains in an otherwise uniform hexagonal microstructure. Figure 5.16 shows the microstructural evolution during the creep deformation simulation of a microstructure containing total of 495 grains and two large grains with $A_{\text{Inhom}}/A_{\text{Hex}} = 8.0$. Observations quite similar to previous simulation results could be made here. Grain-switching events can be clearly observed exactly at the interface of the inhomogeneity and the uniform matrix at 40 % strain value. A close observation of the structure at 70 % strain would reveal that the structure is divided into several regions with grains having horizontal and vertical grain boundaries. This can be attributed to the stress interactions induced by presence of the three larger grains. As observed earlier, these regions are categorized along the diagonal paths originating from the inhomogeneities themselves. More number of perpendicular boundaries at higher strains implies lower stresses and the consequent widening of the strain rate peak.
Figure 5.16: Snapshots showing the structural evolution during the creep deformation of a 495 grains microstructure with three large grains at center and $A_{\text{Inhom}}/A_{\text{Hex}} = 8.0$.

Figure 5.17 shows the normalized strain rates for six such non-uniform microstructures plotted against the strain rate for the regular homogeneous microstructure [42]. The area of one large grain, $A_{\text{Inhom}}$ in the non-uniform microstructure is: 2.0, 4.0, 6.0, 8.0, 10.1 and 16.1
times larger than the area of a hexagonal grain $A_{\text{Hex}}$. Presence of three larger grains has a very significant affect on the strain-rate peak lowering and its consequent broadening. Also, the peak shift towards lower strains is very pronounced in this structure. Comparing the strain-rate peaks for microstructure with one large grain and the one with three large grains i.e. Figure 5.13 and 5.17, it can be easily noticed that the peak value for the area ratio of 12.1 for one-large grain is approximately similar to the peak value for area ratio 4.0 for three-large grain structure. This signifies the inhomogeneity size effect on the strain-rate.

Thus, on the whole, it can be concluded that the increase in the number and size of inhomogeneity in a microstructure removes the singularity and significantly lowers the strain rate. This conclusion can be further validated by comparing the strain rates of different microstructures with increasing number of inhomogeneities and keeping $A_{\text{Inhom}}/A_{\text{Hex}}$ as constant. Figure 5.18 shows one such comparison at a constant area ratio of 8.0. Another similar comparison is shown in Figure 5.19 keeping area ratio constant as 10.0.
Figure 5.18: Normalized stain rate vs. strain for three non-uniform microstructures with varying number of inhomogeneities and at constant area ratio, $A_{\text{Inhom}}/A_{\text{Hex}} = 8.0$, plotted against the strain rate for homogeneous structure.

Figure 5.19: Normalized stain rate vs. strain for three non-uniform microstructures with varying number of inhomogeneities and at constant area ratio, $A_{\text{Inhom}}/A_{\text{Hex}} = 10.0$, plotted against the strain rate for homogeneous structure.
From these two comparisons, it can be clearly seen that an increase in the number of inhomogeneity or larger grains not only lowers the strain rate peak, but also broadens it and shifts towards lower strains. Increase in the size of inhomogeneity also has similar affect on strain-rate. Both of these phenomenon can be attributed to a single observation from the microstructure: increase in the number of horizontal boundaries in preferred diagonal directions or alternatively, decrease in the number of grain-switching events.
6. Conclusions

The present study can be summarized with following conclusions:

1. At elevated temperatures, during superplastic deformation, stress concentrations in a microstructure along a grain boundary path are located at the center of grain boundary segments rather than at the nodes.

2. High normal stress concentrations, close to 3.7 times the applied stress were found on some grain boundary segments in one particular inhomogeneity distribution.

3. Higher amplitudes of stress distributions were found along the paths intersecting inhomogeneities than along other paths which do not intersect the inhomogeneities.

4. Compressive stresses were found to be higher on the grain boundaries surrounding the inhomogeneities as compared to the ones elsewhere in the matrix.

5. Presence of small grains in the microstructure results in increase in stress amplitude on the grain boundary segments in its vicinity.

6. Presence of inhomogeneity in the microstructure removes the singularity in the strain rate.

7. The height of peak in the strain rate decreases with the increase in the size of inhomogeneity.

8. Breaking of inhomogeneity results in peak shift to the left i.e. higher strain rates at lower strains.
References

Appendix A: Analytical Details

This study is based on the Coble Creep deformation at the mesoscale level in two-dimensional systems. The inspirational tool for these simulations has been the pioneering work of Pan and Cocks [41-46]. As per the Pan and Cocks [42] formulation, this work is focused on the deformation mechanism governed by grain-boundary sliding accommodated by grain-boundary diffusion.

GB Diffusion is supposed to be the rate controlling process which leads to the assumption that there is no resistance to relative sliding along the grain-boundaries. Other assumptions are that elastic displacements are ignored and deformation results from the free sliding of grain boundaries accommodated by the diffusional transport of material around the grains.

Figure A.1: Simulation cell consisting of homogeneous grains subjected to axial stress $\sigma_o$.

Figure A.2: Schematic representation of diffusion along the boundary (J) and relative sliding leading to change in grain-boundary thickness $\delta$. 
A.1 Governing Equations

According to the Fick’s Law, the diffusive flux $J$ defined as volume of matter flowing across unit area perpendicular to the flux direction per unit time, is linearly dependent on the gradient of the chemical potential $\mu$ of the diffusing species.

Along the grain boundary, the gradient of the atomic potential is induced by the gradient of stress $\sigma$ acting normal to the boundary.

$$J = \frac{D_{gb} \frac{\partial \Omega}{\partial \sigma_n}}{kT} \frac{\partial \sigma_n}{\partial \delta} \quad (A.1)$$

The excess chemical potential of an atom in the boundary:

$$\mu = -\sigma \Omega \quad (A.2)$$

$\sigma$ – Normal stress acting on the boundary.

$\Omega$ – Atomic volume.

As matter is deposited onto (or removed from) a grain boundary, the two grains determining the grain boundary move apart (towards each other) with a relative normal velocity $v_n$. Conservation of matter requires that:

$$\frac{\partial J}{\partial \delta} + v_n = 0 \quad (A.3)$$

If $J_a > J_b$, i.e. more material gets into this grain boundary segment, than it gets out, then for this single model:

$$v_n + \frac{J_b - J_a}{L} = 0$$

$$v_n = \frac{J_a - J_b}{L} \quad (A.4)$$

Figure A.3: Schematic representation of grain-boundary sliding accommodated by diffusion.
In addition to this, at each junction, where a number, \( m \), of grain-boundaries meet, the flux \( J \) must satisfy the condition:

\[
\sum_{i=1}^{m} \vec{J}_i \cdot \vec{t}_i = 0
\]  \hspace{1cm} (A.5)

where, \( \vec{J}_i \) is the flux into boundary \( i \) and \( \vec{t}_i \) is a unit vector in the direction of the \( i \)-th boundary pointing away from the boundary.

![Image of flux movement to show mass conservation across a node.](image)

**Figure A.4:** Flux movement to show mass conservation across a node.

![Image of schematic representation of degrees of freedom in the system.](image)

**Figure A.5:** Schematic representation of degrees of freedom in the system.
A.1.1 Variational Principle

Needleman and Rice [1980] have shown that the solution of the above set of coupled equations is provided by the set of centers of mass velocities (both translational and rotational) and by the flux pattern (flux value of the center of each GB segment) which minimizes the functional:

$$\Pi = \int_s \frac{kT}{2D_{gb}} J^2 ds - \int_{\Gamma} T_{a} V_{a} d\Gamma + \sum_{\text{vertices}} \lambda_n (\sum_{\text{rays}} J)$$  \hfill (A.6)

The Lagrange multiplier is introduced to include the boundary condition of mass conservation at triple points. No cavities or voids are assumed in this model. Therefore, the degrees of freedom are: \{v_x, v_y\}, {\omega}, {\lambda}, {J}.

A.1.2 Normalized Units Formulation

One can consider d as a suitably defined mean grain size and \(\sigma_0\) as a suitable normalizing stress. Using these, the following normalizations are adopted:

- Distances: \(\tilde{s} = \frac{s}{d}\)
- Traction (force per unit length): \(\tilde{T}_{a} = \frac{T_{a}}{\sigma_0}\)
- Velocity: \(\tilde{V}_{a} = \frac{V_{a}}{\dot{\varepsilon}_o d}\); Angular Velocity: \(\tilde{\omega} = \frac{\omega}{\dot{\varepsilon}_o}\)
- Time: \(\tilde{t} = \frac{t}{1/\dot{\varepsilon}_o} = \dot{\varepsilon}_o t\) where \(\dot{\varepsilon}_o = \frac{D_b\delta\Omega\sigma_0}{kTd^3}\)

(The reference typical strain rate \(\dot{\varepsilon}_o^{-1}\) is used to define the unit of time)
- Flux (Volumetric flux of matter): \(\tilde{J} = \frac{J}{\dot{\varepsilon}_o d^2}\)
- Normal Stress: \(\tilde{\sigma}_n = \frac{\sigma_n}{\sigma_0}\)
- Lagrange Multipliers: \(\tilde{\lambda}_n = \frac{\lambda_n}{\sigma_0}\)

Adopting this reduced units representation, we can write:

$$\overline{\Pi} = \frac{1}{2} \int_s \tilde{J} \tilde{J} ds - \int_{\Gamma} \tilde{T}_{a} \tilde{V}_{a} d\Gamma + \sum_{\text{vertices}} \tilde{\lambda}_n (\sum_{\text{rays}} \tilde{J})$$ \hfill (A.8)
where the normalized power is: \[ \bar{\Pi} = \frac{\Pi}{\dot{\varepsilon}_o \sigma_o d^2} \]

### A.2 Evaluation of the Dissipative Terms

To evaluate the dissipation due to the diffusional creep on GB segment, let us select a typical grain-boundary segment (in this case, the entire GB) separating grains 1 and 2 (Figure A.6).

![Figure A.6: Grain boundary element showing local coordinate and degrees of freedom](image-url)

Figure A.6: Grain boundary element showing local coordinate and degrees of freedom [42].
(a) First, define the local coordinates along the selected GB element. Define the normal to the GB element \( \mathbf{n}^e \) with the components \( n_x^e \) and \( n_y^e \) in the global coordinate system. There are two possible choices for the direction of this normal and one can choose any of them. However, as soon as the normal direction is decided upon, the local coordinate system along the grain boundary is always chosen so that its origin is located at the mid-point of the grain facet and its positive direction makes an angle 90° anti-clockwise with respect to the normal. The grain on the tail side of the normal is always referred to as the first grain with respect to the GB element and similarly the grain on the head side of the normal is always referred to as the second grain with respect to the grain boundary.

(b) Define the center of the grain as the point whose coordinates are equal to the mean of the coordinates of the mid-points of the facets that encircle the grain.

\[
\begin{align*}
    x_c &= \frac{\sum_{i=1}^{5} x_i}{5} \\
    y_c &= \frac{\sum_{i=1}^{5} y_i}{5}
\end{align*}
\]  

(A.9)

Figure A.7: Coordinates of the grain-center and the centers of the surrounding facets.
The degrees of freedom associated with a grain-boundary element are:
- The velocities associated with the centers of the two grains involved i.e. \( v_{x1}, v_{y1}, v_{x2}, v_{y2} \). (4 nos.)
- The angular velocities of the two grains i.e. \( \omega_1, \omega_2 \). (2 nos.)
- The value of diffusive flux, \( J_o \) in the center of the GB segment. (1 no.)
- The values of \( \lambda_n \) called \( \sigma^+ \) and \( \sigma^- \) at the positive and negative ends of the element. (2 nos.)

Total 9 degrees of freedom: \( [v_{x1}, v_{y1}, v_{x2}, v_{y2}, \omega_1, \omega_2, J_o, \sigma^+, \sigma^-] \) \hfill (A.10)

Knowing the velocities of centers of mass of each of the two grains \{ \( v_{x1}, v_{y1}, \omega_1 \) \} and \{ \( v_{x2}, v_{y2}, \omega_2 \) \}, positions of the centers of mass of the two grains, position of the face center, and the components of the normal vector to the interface, the velocity along the GB segment can be written as:

\[
V(s) = [B_o] [U_o] \hfill (A.11)
\]

Where, \( V(s) \) is the relative velocity with which grains either side move apart,

\[
[B_o] = [-n_x, -n_y, (s+l_1), n_x, n_y, -(s+l_2)] \hfill (A.12)
\]

and

\[
[U_o] = [v_{x1}, v_{y1}, \omega_1, v_{x2}, v_{y2}, \omega_2]^T = \begin{bmatrix} v_{x1} \\ v_{y1} \\ \omega_1 \\ v_{x2} \\ v_{y2} \\ \omega_2 \end{bmatrix} \hfill (A.13)
\]

Here, \( l_1 \) – is the negative value of the local coordinate where a line drawn parallel to \( \hat{n}^e \) through the center of the first grain intersects the GB facet (Figure A.6).

and, \( l_2 \) – is the negative value of the local coordinate where a line drawn parallel to \( \hat{n}^e \) through the center of the second grain intersects the GB facet (Figure A.6).
A.2.1 Proof of Relations A.11, A.12 and A.13

Given a point along the GB separating the two grains, the normal velocity with which the two sides of the boundary move apart can be calculated by considering the fact that the two grains move relative to the global coordinate system with translational velocities \( (v_{xi}, v_{yi}; i=1, 2) \) and angular velocities \( (\omega_i; i=1, 2) \) i.e. rotation.

(a) First, we analyze the effect due to the rotation of the two grains. Assuming that the Grain 1 (say) only rotates with the angular velocity \( \omega_1 \) (perpendicular to the figure), then the velocity of a point P located on the GB, by \( \vec{r}_1 \) from the grain center is given by:

\[
\vec{v}_1^{\text{rot}} = \omega_1 \times \vec{r}_1
\]

The component of this velocity parallel to \( \vec{n} \) (the normal unit vector to the boundary) gives the separation velocity:

\[
v_{1n} = \vec{v}_1^{\text{rot}} \cdot \vec{n}
\]

In a similar way, we can define the same quantities for second grain:

\[
\vec{v}_2^{\text{rot}} = \omega_2 \times \vec{r}_2
\]

\[
v_{2n} = \vec{v}_2^{\text{rot}} \cdot \vec{n}
\]

Using these quantities, we can define the velocity with which the boundaries move apart as:

\[
v^{\text{rot}}(s) = v_{1n}^{\text{rot}} - v_{2n}^{\text{rot}} = \left( \omega_1 \times \vec{r}_1 \right) \cdot \vec{n} - \left( \omega_2 \times \vec{r}_2 \right) \cdot \vec{n}
= \omega_1 \left( \vec{r}_1 \times \vec{n} \right) - \omega_2 \left( \vec{r}_2 \times \vec{n} \right)
= \omega_1 \left( l_1 + s \right) - \omega_2 \left( l_2 + s \right)
\]

Where \( \left( \vec{r}_1 \times \vec{n} \right) \) represents the component of \( \vec{r}_1 \) along the s-axis parallel to the GB in local coordinate system.

It is assumed in this analysis that the coordinates along the GB are measured with respect to local coordinate system which measure s along the GB from the middle of GB by knowing the coordinate of point P and \( l_1 \) and similarly with \( l_2 \).

(b) Analyze the effect of grains translating with respect to each other.
Locally, for example, due to translation of the first grain, the velocity at point P is:

\[
\vec{v}_1^{\text{trans}} = v_{x1} \vec{x} + v_{y1} \vec{y}
\]

The normal component of this is:

\[
\vec{v}_{1n}^{\text{trans}} = \vec{v}_1^{\text{trans}} \cdot \vec{n} = v_{x1} n_1 + v_{y1} n_2
\]

Similar rotations are obtained for the side of the GB inside grain 2:

\[
\vec{v}_2^{\text{trans}} = v_{x2} \vec{x} + v_{y2} \vec{y}
\]

\[
\vec{v}_{2n}^{\text{trans}} = \vec{v}_2^{\text{trans}} \cdot \vec{n} = v_{x2} n_1 + v_{y2} n_2
\]
The relative separation due to these two grains is given by:

\[ v_{\text{trans}}^\text{trans}(s) = v_{2\text{n}}^\text{trans} - v_{1\text{n}}^\text{trans} \]
\[ = -v_{x1}n_1 - v_{y1}n_2 + v_{x2}n_1 + v_{y2}n_2 \]

(c) Combining both grain rotation and grain translation gives the separation velocity:

\[ v(s) = v_{\text{rot}}(s) + v_{\text{trans}}^\text{trans}(s) \]

\[ v(s) = -v_{x1}n_1 - v_{y1}n_2 + v_{x2}n_1 + v_{y2}n_2 + \omega_1(l_1 + s) - \omega_2(l_2 + s) \]  \( \text{(A.14)} \)

Equation A.14 is same as Equations A.11-A.13 as derived in [42]

A.2.2 Solution of Equations

Knowing the separation velocity \( [v(s)] \) along an interface, the continuity equation (in terms of volume conservation) gives:

\[ \frac{\partial J}{\partial s} + v(s) = 0 \]  \( \text{(A.15)} \)

Integrating this:

\[ J(s) = \int_0^s -v(s)ds + J_o = -\int_0^s [B_o(s)][U_o]ds + J_o \]

\[ = \left\{ -\int_0^s [B_o(s)]ds \right\}[U_o] + J_o \]

Including \( J_o \) as another degree of freedom vector \( [U_o] \), this become \([U]\):

where:

\[ [U] = [v_{x1} \quad v_{y1} \quad \omega_1 \quad v_{x2} \quad v_{y2} \quad \omega_2 \quad J_o]^T \]  \( \text{(A.16)} \)

Figure A.8: Separation velocity and local coordinates of the GB element
Then by integrating \(-\int_0^s[B(s)]ds\) and adding one more element, we get \([B]\)

\[
[B] = \begin{bmatrix}
n_1s & n_2s & -\left(0.5s^2 + l_1s\right) & n_1s & -n_2s & \left(0.5s^2 + l_2s\right)
\end{bmatrix}
\]  

(A.17)

With this we can write

\[
J(s) = [B][U]
\]  

(A.18)

Now we can evaluate the contribution of the dissipation from this GB element. This is given by:

\[
\frac{1}{2} \int_{-\frac{L}{2}}^{+\frac{L}{2}} J^2(s)ds = \frac{1}{2} \int_{-\frac{L}{2}}^{+\frac{L}{2}} J\cdot J ds = \frac{1}{2} \int \left[B^\top[U][U] + [B][U]ds \right. \\
= \frac{1}{2} \left[2\int J^2(s)ds = \frac{1}{2} [U^\top][K][U] \right. \\
\]  

(A.19)

where, \([K]\) is the viscous matrix given by:

\[
[K] = \int_{-\frac{L}{2}}^{+\frac{L}{2}} [B]^\top[B] ds
\]  

(A.20)

Explicit form of Equation A.20 is given by the formula derived in the Appendix of [42].

The matrix \([K]\) given in Equation A.20 can be viewed as the product of the elements of vector \([B]\). In terms of matrix elements this can be written as:

\[
K_{ij} = \int B_i B_j ds
\]  

(A.21)

where, \(i, j = 1, 7\) and \([K]\) is a symmetric 7X7 matrix.

Equation A.21 can be derived from A.19 by writing it in the matrices component form:

\[
\frac{1}{2} \int_{-\frac{L}{2}}^{+\frac{L}{2}} J^2(s)ds = \frac{1}{2} \int_{-\frac{L}{2}}^{+\frac{L}{2}} \left( \sum_{i=1}^{7} B_i U_i \right) \left( \sum_{j=1}^{7} B_j U_j \right) ds = \frac{1}{2} \int_{-\frac{L}{2}}^{+\frac{L}{2}} \left( \sum_{i,j=1}^{7} B_i B_j ds U_i U_j \right) \\
= \frac{1}{2} \left( \sum_{i,j=1}^{7} \int_{-\frac{L}{2}}^{+\frac{L}{2}} (B_i(s)B_j(s)ds) \right) U_i U_j = \frac{1}{2} \sum_{i,j=1}^{7} K_{ij} U_i U_j = \frac{1}{2} U^\top K U
\]  

(A.22)
Equation A.22 can be written in matrix form by introducing a symmetric matrix \([K]\), whose elements are defined in A.22 itself:

\[
[K] = 
\begin{bmatrix}
    n_1^2s' & n_1n_2s' & -n_1l_1s' & -n_1n_2s' & n_1l_2s' & 0 \\
    n_2^2s' & -n_2l_1s' & -n_1n_2s' & -n_2^2s' & n_2l_2s' & 0 \\
    0.1\left(\frac{L}{2}\right)^5 + l_1^2s' & n_1l_1s' & n_2l_1s' & -0.1\left(\frac{L}{2}\right)^5 - l_1l_2s' & -0.5s' \\
    n_1^2s' & n_1n_2s' & -n_1l_2s' & 0 \\
    n_2^2s' & -n_2l_2s' & 0 \\
    0.1\left(\frac{L}{2}\right)^5 + l_2^2s' & +0.5s' & 2\left(\frac{L}{2}\right)
\end{bmatrix}
\]

In Equation A.23, \(s'\) is given by:

\[
s' = \int_{-\frac{L}{2}}^{\frac{L}{2}} s^2 ds = \frac{2}{3}\left(\frac{L}{2}\right)^3
\]

\[\text{(A.24)}\]

A.2.3 Application of Mass Conservation

![Figure A.9: Lagrange Multiplier terms to impose mass conservation.](image)

Referring to Figure A.9, if \(\sigma_n^+\) and \(\sigma_n^-\) are the values of \(\lambda_n\) at the positive and negative ends of the element then the generic term, \(\sum_{\text{vertices}} \left(\lambda_n \sum_{\text{rays}} J\right)\) for the GB segment reduces to:
\[
\begin{bmatrix}
\sigma_n^+ & \sigma_n^- \\
\end{bmatrix}
\begin{bmatrix}
J(s = +\frac{L}{2}) \\
-J(s = -\frac{L}{2}) \\
\end{bmatrix} = [\lambda]'^T[C][U]
\]  

(A.25)

where, \([\lambda] = [\sigma_n^+ \quad \sigma_n^-]^T\) and \([C]\) are given in Appendix of [42].

The explicit expression for the elements of matrix \([C]\) can be derived by using Equation A.18 and finding the explicit values of the GB diffusional flux currents at \(s = -L/2\) and \(s = L/2\).

Using Equation A.18:

\[
J\left(s = \frac{L}{2}\right) = \begin{bmatrix}
n_1 \frac{L}{2} & n_2 \frac{L}{2} & -\left(0.5 \left(\frac{L}{2}\right)^2 + l_1 \frac{L}{2}\right) & -n_1 \frac{L}{2} & -n_2 \frac{L}{2} & \left(0.5 \left(\frac{L}{2}\right)^2 + l_2 \frac{L}{2}\right) & 1 & [U] \\
\end{bmatrix}
\]

\[
J\left(s = -\frac{L}{2}\right) = \begin{bmatrix}
-n_1 \frac{L}{2} & -n_2 \frac{L}{2} & -\left(0.5 \left(\frac{L}{2}\right)^2 - l_1 \frac{L}{2}\right) & +n_1 \frac{L}{2} & +n_2 \frac{L}{2} & \left(0.5 \left(\frac{L}{2}\right)^2 - l_2 \frac{L}{2}\right) & 1 & [U] \\
\end{bmatrix}
\]

\[
\ldots\ldots(A.26)
\]

Therefore, combining A.25 and A.26, we get:

\[
\begin{bmatrix}
\sigma_n^+ & \sigma_n^- \\
\end{bmatrix}
\begin{bmatrix}
J(s = +\frac{L}{2}) \\
-J(s = -\frac{L}{2}) \\
\end{bmatrix} = [\lambda]'^T[C][U]
\]

with:

\[
[C] = \begin{bmatrix}
n_1 \frac{L}{2} & n_2 \frac{L}{2} & -\left(0.5 \left(\frac{L}{2}\right)^2 + l_1 \frac{L}{2}\right) & -n_1 \frac{L}{2} & -n_2 \frac{L}{2} & \left(0.5 \left(\frac{L}{2}\right)^2 + l_2 \frac{L}{2}\right) & 1 \\
n_1 \frac{L}{2} & n_2 \frac{L}{2} & \left(0.5 \left(\frac{L}{2}\right)^2 + l_1 \frac{L}{2}\right) & -n_1 \frac{L}{2} & -n_2 \frac{L}{2} & \left(0.5 \left(\frac{L}{2}\right)^2 + l_2 \frac{L}{2}\right) & -1 \\
\end{bmatrix}
\]

(A.27)

Important: In Pan and Cocks [42], this constraint matrix is given by (-1)[C]. This might be because of the different convention for the mass conservation at a triple point. They might have considered all the currents coming out of a node as positive instead of assuming all currents going into a node to be positive. Maintaining either convention in a consistent manner would be fine.
Note: When considering all the GB elements of the microstructure, all the sums over triple junctions can be recovered. \( \lambda_n \sum_{\text{rays}} \). It is assumed here that no voids or cracks are present in the system.

A.2.4 Application of External Traction
Applying external traction on the system can be done by writing \(- \int T_\alpha V_\alpha ds\) for a GB along which a traction \( T_\alpha \) is exerted (normal to the GB segment). In the beginning, forces will be applied only on the edges the simulation cell and parallel to the axes of coordinates. Therefore, for each GB element, we can estimate the contribution from the applied tractions \( T=\sigma \) and can write \( T.V \) as \([F].[U]\). The expression for GB velocities is expressed in terms of velocities at the center of the grains adjacent to the specimen boundary and therefore as a function of \([U]\).

In the end, by adding the two more degrees of freedom for the stresses normal to the grain boundaries, there are 9 degrees of freedom for each GB element as mentioned in Equation A.10. Using this, a general stiffness matrix \([G]\) can be assembled using \([K]\), given by Equation A.23 and \([C]\) given by Equation A.27. Similarly, a traction matrix \([F]\) and the global matrix \([U]\) of degrees of freedom and constraints can be formed. Thus,
\[ \pi = \frac{1}{2} \left[ U \right]^T \left[ G \right] \left[ U \right] - \left[ F \right] \left[ U \right] \]  
(A.28)

Taking the variation \( \delta \pi = 0 \), gives:
\[ [G] [U] = [F] \]  
(A.29)

or
\[ [U] = [G]^{-1} [F] \]  
(A.30)

Equation A.29 and A.30 can be solved using standard numerical matrix methods like Crout’s factorization.
Appendix B: Imposing Boundary Conditions

B.1 Degrees of Freedom Associated with Grains

Figure B.1 represents a microstructure with all four boundaries as axis of symmetry, such that the part of the microstructure shown represents a repeating unit within an infinite body. The three degrees of freedom associated with each grain are: \( \{v_x, v_y, \omega_i\} \). However, to eliminate the rigid body motion and to satisfy the condition that each grain bordering one of the symmetry axes is not rotating, some constraints need to be imposed.

![Figure B.1: Microstructure containing 18 grains with different degrees of freedom.](image)

It can be observed from the figure that only four grains marked as 6, 7, 8 and 10 respectively (completely inside the simulation box) have degree of freedom associated with the rotation motion. The grains with their center on the simulation box or having at least one side on the simulation box, do not have rotational degrees of freedom. The grains in the microstructure can be divided into three more groups:
1) Grains which have their centers inside the simulation box and also a side bordering the boundary of simulation cell. These grains have only 2 degrees of freedom \(\{v_x, v_y, \omega=0\}\).

2) Grains which have their center on the boundary AB and BC (\(x=\text{box}_x, y=\text{box}_y\)) of simulation cell and only a part of the grain is inside the simulation cell. These grains have 2 degrees of freedom, associated with translation motion \(\{v_x, v_y, \omega=0\}\).

3) Grains which have their center located on the axis, \(x=0\) and \(y=0\) and only a part of the grain is inside the simulation cell. These grains have only 1 degree of freedom:
   - Those on the \(x=0\) axis have \(\{v_x=0, v_y, \omega=0\}\).
   - Those on the \(y=0\) axis have \(\{v_x, v_y=0, \omega=0\}\).

### B.2 Degrees of Freedom Associated with Grain Boundaries

It is now necessary to identify the degrees of freedom associated with all real grain boundaries of the microstructure. Owing to the periodic boundary conditions, the grain boundaries are divided into three categories:

1) Regular boundaries that are entirely inside the simulation cell (Figure B.2 (a)) have a diffusional current, \(J_i\), passing through middle of them, taken as degree of freedom \(\{J_i\}\). The thickness associated with these boundaries is \(\delta\).

2) Half-boundaries located along the axis of symmetries and separating two distant grains. These boundaries do have a diffusional current along them and the value at the center is taken as degree of freedom \(\{J_i\}\). However, in calculations, the thickness of these boundaries is taken as \(\delta/2\). This results in a multiplication factor of 2 for some of the terms in stiffness matrix.

3) Quasi grain boundaries (marked as dotted in Figure B.2 (b)) are only apparent boundaries. They are located on the boundary of simulation cell and by symmetry are ‘inside’ the grains. They do not have any degrees of freedom associated with them.

![Diagram](image_url)

Figure B.2: Differentiating between the different types of boundaries in the simulation cell.
B.3 Degrees of Freedom Associated with Triple Junctions

Imposing mass conservation implies that the fluxes of matter entering or leaving a node have to be conserved. In variational formulation, each node is assigned a degree of freedom \( \{\sigma_c\} \) (Lagrange Multiplier). \( \sigma_c \) is the value of normal stress along all the boundaries meeting at a triple point. There are two types of nodes:

1) Regular nodes through which there is a net flow of material. They have one degree of freedom. These nodes include the regular triple junctions located inside the simulation cell and the nodes located on the simulation cell boundary, having at least one grain-boundary located on the simulation cell boundary, through which there is a net flux of matter.

2) Nodes located on the boundary of the simulation cell, through which there is no net flow of matter. There is no degree of freedom associated with them. These include the corner nodes (considered to be located inside the grains) and boundary nodes for which both boundaries located on the simulation cell are non-active boundaries.
Appendix C: Dissipative Term

The matrix form of the dissipative term: 
\[ \frac{1}{2} \int_{L_{\text{GB}}} J^2(s) ds \] 
for the three types of boundaries in this mesoscopic simulation.

The GBs degree of freedom is given by the vector in (A.16) as:

\[ [U] = [v_{x1} \quad v_{y1} \quad \omega_1 \quad v_{x2} \quad v_{y2} \quad \omega_2 \quad J_0]^T \]  \hspace{1cm} (C.1)

The expression for the diffusion current along the GB at distance s from the GB center is given as:

\[ J(s) = [B(s)][U] \]  \hspace{1cm} (C.2)

where:

\[ [B] = \begin{bmatrix} n_x s & n_y s & -(0.5s^2 + l_1 s) & n_x s & n_y s & (0.5s^2 + l_2 s) & 1 \end{bmatrix} \]  \hspace{1cm} (C.3)

The dissipative term can be calculated over the length of grain boundary L_{GB}, if (C.1) to (C.3) are known. However, in calculating the expression, we have to differentiate between the three types of boundaries as mentioned in Section B.2.

In non-reduced unit, the individual GB dissipative term is written as:

\[ \Pi_{GB} = \frac{kT}{2D_{GB} \delta \Omega_{GB}} \int J^2(s) ds \]  \hspace{1cm} (C.4)

After differentiating the grain boundaries on the basis of their different diffusive width, we can write:

\[ \delta = \frac{1}{\alpha} \delta_b \]  \hspace{1cm} (C.5)

where, \( \delta \) – The actual value of diffusional width
\( \alpha \) – Parameter characterizing each boundary
\( \delta_b \) – The typical value of diffusion width

For regular boundaries with both vertices completely inside simulation cell or the boundaries intersecting the simulation box (Figure E.1) with one vertex inside simulation cell, \( \alpha = 1 \).

For half boundaries (Figure B.2 (b)), which have diffusion width as \( \frac{1}{2} \delta \), \( \alpha = 2 \).

Using the Equation C.4, the dissipative term can be written in reduced unit as:

\[ \Pi^* = \alpha \frac{kT}{2D_{GB} \delta \Omega_{GB}} \int J^2(s) ds = \alpha \Pi_{GB} \]  \hspace{1cm} (C.6)
C.1 Regular Boundary with Both Vertices inside Simulation Cell

For such a boundary:

$$\Pi^* = \frac{1}{2} \int_{GB} J^2(s) ds = \frac{1}{2} \int_{-L/2}^{L/2} \left[ B(s) \right] \left[ U B(s) \right] ds = \frac{1}{2} [U]^T [K] [U]$$  \hspace{1cm} (C.7)

where,

$$K_{ij} = \int_{-L/2}^{L/2} B_i(s) B_j(s) ds$$  \hspace{1cm} (C.8)

Using Equation C.3, substituting for vector B and integrating along the grain boundary, we obtain:

$$[K] = \begin{bmatrix}
  n_z^2 s' & n_x n_y s' & -n_z l_1 s' & -n_x n_y s' & n_x l_2 s' & 0 \\
  n_y^2 s' & -n_y l_1 s' & -n_x n_y s' & -n_y^2 s' & n_y l_2 s' & 0 \\
  0.1 \left( \frac{L}{2} \right)^5 + l_2^2 s' & n_x l_1 s' & n_y l_1 s' & -\left( 0.1 \left( \frac{L}{2} \right)^5 + l_1 l_2 s' \right) & -0.5 s' \\
  n_z^2 s' & n_x n_y s' & -n_z l_1 s' & 0 \\
  n_y^2 s' & -n_y l_1 s' & -n_x n_y s' & 0 \\
  0.1 \left( \frac{L}{2} \right)^5 + l_2^2 s' & 0 & 0 & 2 \left( \frac{L}{2} \right)
\end{bmatrix}$$  \hspace{1cm} (C.9)

Here, $s' = \int_{-L/2}^{L/2} s^2 ds = \frac{2}{3} \left( \frac{L}{2} \right)^3$

Note: For boundaries of various diffusivities, all the elements of matrix $[K]$ have to be multiplied by a constant, affecting the diffusivity.
C.2 Half Regular Boundary with Both Vertices on Simulation Cell

The reduced functional term will be exactly same as that given by Equation E.9. However, the diffusive width of this boundary is only half of a regular boundary. So, we will account for $\alpha=2$ here.

$$[K] \rightarrow \alpha[K]$$

C.3 Regular Boundary with One Vertex on Simulation Cell

For this grain boundary, components of the matrix $[K]$ have to be reevaluated.

For $v_1$ on the boundary

$$K_{11} = \begin{cases} \int_0^L B_1(s)B_1(s)ds = n_x^2 \int_0^L s^2 ds = n_x^2 \frac{L^3}{3} & \text{For } v_1 \text{ on the boundary} \\ \int_{-L}^0 B_1(s)B_1(s)ds = n_x^2 \int_{-L}^0 s^2 ds = n_x^2 \frac{L^3}{3} & \text{For } v_2 \text{ on the boundary} \end{cases}$$

$$K_{12} = n_x n_y \frac{L^3}{3}$$

For $v_1$ on the boundary

$$K_{13} = \begin{cases} -n_x \int_0^L [0.5s^3 + l_1 s^2] ds = -n_x \left[ 0.5 \frac{L^4}{4} + l_1 \frac{L^3}{3} \right] & \text{For } v_1 \text{ on the boundary} \\ -n_x \int_{-L}^0 [0.5s^3 + l_1 s^2] ds = -n_x \left[ -0.5 \frac{L^4}{4} + l_1 \frac{L^3}{3} \right] & \text{For } v_2 \text{ on the boundary} \end{cases}$$

$$K_{14} = -n_x^2 \frac{L^3}{3}$$

Figure E.1: Regular boundary with one vertex on simulation cell
\[
K_{15} = -n_x n_y \frac{L^3}{3}
\]

\[
K_{16} = \begin{cases} 
  n_x \left[ 0.5 \frac{L^4}{4} + l_2 \frac{L^3}{3} \right] & \text{For } v_1 \text{ on the boundary} \\
  n_x \left[ -0.5 \frac{L^4}{4} + l_2 \frac{L^3}{3} \right] & \text{For } v_2 \text{ on the boundary}
\end{cases}
\]

\[
K_{17} = \begin{cases} 
  n_x \frac{L^2}{2} & \text{For } v_1 \text{ on the boundary} \\
  -n_x \frac{L^2}{2} & \text{For } v_2 \text{ on the boundary}
\end{cases}
\]

\[
K_{22} = n_y^2 \frac{L^3}{3}
\]

\[
K_{23} = -n_y \begin{cases} 
  0.5 \frac{L^4}{4} + l_1 \frac{L^3}{3} & \text{For } v_1 \text{ on the boundary} \\
  -0.5 \frac{L^4}{4} + l_1 \frac{L^3}{3} & \text{For } v_2 \text{ on the boundary}
\end{cases}
\]

\[
K_{24} = -n_x n_y \int s^2 \, ds = -n_x n_y \left( \frac{L^3}{3} \right)
\]

\[
K_{25} = -n_y^2 \int_0^L s^2 \, ds = -n_y^2 \frac{L^3}{3}
\]

\[
K_{26} = n_y \begin{cases} 
  0.5 \frac{L^4}{4} + l_2 \frac{L^3}{3} & \text{For } v_1 \text{ on the boundary} \\
  -0.5 \frac{L^4}{4} + l_2 \frac{L^3}{3} & \text{For } v_2 \text{ on the boundary}
\end{cases}
\]

\[
K_{27} = n_y \frac{L^2}{2}
\]
Appendix D: Stiffness Matrix

It’s already shown in A.18 that for a given GB, the diffusion current can be written as:

\[ J(s) = [B][U] \]

with \([B]\) and \([U]\) given by Equations A.16 and A.17 respectively. Power dissipation term is given by Equation A.19 as:

\[
\frac{1}{2} \int_{-\frac{1}{2}}^{+\frac{1}{2}} J^2(s) ds = \frac{1}{2} [U]^T [K][U]
\]

where \([K]\) is given by Equation A.23. Similarly, the mass conservation term \(\sum_{\text{vertices}} \left( \lambda_n \sum_{\text{rays}} J \right)\) for each GB can be written as \([\lambda]^T[C][U]\) where \([\lambda] = [\sigma^+_n \ \sigma^-_n]^T\) and \([C]\) is given in Equation A.27.

A unified set of degrees of freedom for a certain GB in the microstructure can be defined as:

\[
[U_{GB}] = [v_x1 \ v_y1 \ \omega_1 \ v_x2 \ v_y2 \ \omega_2 \ J_0 \ \lambda_2 \ \lambda_1]^T \quad (D.1)
\]

The contribution to the dissipative function due to a GB can be extended from the general expression

\[
\Pi = \frac{1}{2} \int_{\Gamma} J \Pi d\Gamma - \int_{\Gamma} \bar{T}_\alpha \bar{V}_\alpha d\Gamma + \sum_{\text{vertices}} \bar{\lambda}_n (\sum_{\text{rays}} J)
\]

as:

\[
\Pi_{GB} = (1/2) [U_{GB}]^T [A_{GB}] [U_{GB}] \quad (D.2)
\]

where,

\[
[A_{GB}] = \begin{bmatrix} K & C^T \\ C & 0 \end{bmatrix} \quad (D.3)
\]

\([A_{GB}]\) represents the generalized viscosity matrix for the grain-boundary diffusion element, with \([K]\) and \([C]\) given by Equation A.23 and A.27 respectively.

The contribution of external forces applied along certain boundaries (GBs) to the variational functional can be written as:

\[- [F_{GB}][U_{GB}]\]

where \([U_{GB}]\) is the unknown elementary vector for the GB, where there is externally applied force and \([F_{GB}]\) is the generalized applied force.
Example: If the applied force is an externally applied stress of value $\sigma$, on the GB located along the simulation cell boundary, acting along the direction $\hat{f}$, then:

$$
-\int_{-L_{GB}/2}^{L_{GB}/2} \vec{F} \cdot \vec{v} = -\sigma \cdot L_{GB} \cdot \vec{v} \cdot \hat{f}
$$

The component of $\hat{f}$ in $\vec{y}$ direction represents the externally applied stress and that in $\vec{x}$ is the stress either along $O_x$ or $O_y$ direction. The velocity along the GB is same as that of the center of the grain determining the GB.

In the simulation, if the external stress is applied only along $O_y$ axis, then for a given boundary located along the axis $y=\text{box}_y$, the force term will be: $-\sigma \cdot L_{GB} \cdot v_{cy}$.

Therefore if, $[U]^T = [v_{x1} \ v_{y1} \ \omega_1 \ v_{x2} \ v_{y2} \ \omega_2 \ \ J_0 \ \lambda_2 \ \lambda_1]$ for the GB, where the force is applied, then

$$
[F] = [0 \ +\sigma L_{GB} \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]
$$

Assembling the global viscosity matrix and force matrix, one can write:

$$
\Pi = \frac{1}{2} [U]^T [A] [U] - [F] [U]
$$

Taking the variation, $\delta \Pi^* = 0$,

$$
[A] [U] = [F]
$$

or,

$$
[U] = [A^{-1}] [F]
$$
Appendix E: Stress Calculation

Stress normal to a grain boundary (GB) can be calculated, once the degrees of freedom associated with the GB (i.e. \([U]\)) are known. The flux of vacancies along each boundary can be given by:

\[
J(s) = [B] [U] \tag{E.1}
\]

where,

\[
[B] = [n_1\bar{s} \quad n_2\bar{s} \quad -\left(0.5\bar{s}^2 + l_3\bar{s}\right)\quad -n_1\bar{s} \quad -n_2\bar{s} \quad \left(0.5\bar{s}^2 + l_3\bar{s}\right) \quad 1] \tag{E.2}
\]

\[
[U] = [v_{x_1} \quad v_{y_1} \quad \omega_1 \quad v_{x_2} \quad v_{y_2} \quad \omega_2 \quad J_0]
\]

Also,

\[
J = \frac{D_{GB}\partial \Omega}{kT} \frac{\partial \sigma}{\partial \bar{s}} \tag{E.3}
\]

In reduced units (normalized units), we get:

\[
\bar{J}\bar{\dot{e}}_o d^2 = \frac{D_{GB}\partial \Omega \sigma_o}{kTd} \frac{\partial \sigma}{\partial \bar{s}}
\]

If, \(\dot{e}_o = \frac{D_{h}\partial \Omega \sigma_o}{kTd^3}\), then we get: \(\bar{J} = \frac{d\sigma}{d\bar{s}}\)

Integrating, we get:

\[
\sigma = \int_{-\bar{s}_o}^{\bar{s}} Jd\bar{s} + \lambda_1
\]

\[
\sigma(\bar{s}) = \lambda_1 + \int_{-\bar{s}_o}^{\bar{s}} Jd\bar{s}\tag{E.4}
\]

where, \(s_o = (1/2)L_{GB}\)

Using Equation E.3., we get:

\[
\sigma(\bar{s}) = \lambda_1 + [D][U] \tag{E.5}
\]

where:

\[
[D] = \begin{bmatrix}
\frac{1}{2} s^2 - \left(\frac{L}{2}\right)^2 & s^2 - \left(\frac{L}{2}\right)^2 & -\frac{s^3}{6} + l_1 \frac{s^2}{2} + \frac{1}{6} \left(\frac{L}{2}\right)^3 - \frac{l_1}{2} \left(\frac{L}{2}\right)^2 \\
\frac{1}{2} s^2 - \left(\frac{L}{2}\right)^2 & \frac{1}{2} s^2 - \left(\frac{L}{2}\right)^2 & -\frac{s^3}{6} + l_1 \frac{s^2}{2} + \frac{1}{6} \left(\frac{L}{2}\right)^3 - \frac{l_1}{2} \left(\frac{L}{2}\right)^2
\end{bmatrix} \tag{E.6}
\]
The total normal traction along a GB can be evaluated, once $\bar{\sigma}(s)$ is known.

$$T_{GB} = \frac{l}{\bar{\sigma} \frac{\lambda}{L}} + \left\{ \int \left[ D(\bar{\sigma}) \right] d\bar{\sigma} \right\} \left[ U \right]$$

$$T_{GB} = \lambda_1 L + [H][U]$$

Where vector $[H]$ components are given by:

$$[H] = \int \frac{l}{\bar{\sigma} \frac{\lambda}{L}} \left[ D(\bar{\sigma}) \right] d\bar{\sigma}$$

$$[H] = \left[ \begin{array}{c}
\frac{n_x}{2} \left( \frac{2}{3} \left( \frac{L}{2} \right)^3 - L \left( \frac{L}{2} \right)^2 \right) \\
\frac{n_y}{2} \left( \frac{2}{3} \left( \frac{L}{2} \right)^3 - L \left( \frac{L}{2} \right)^2 \right) \\
\frac{n_z}{2} \left( \frac{2}{3} \left( \frac{L}{2} \right)^3 - L \left( \frac{L}{2} \right)^2 \right)
\end{array} \right] - \left\{ \frac{l_1}{2} \left( \frac{2}{3} \left( \frac{L}{2} \right)^3 \right) + \left( \frac{1}{6} \left( \frac{L}{2} \right)^3 - \frac{l_1}{2} \left( \frac{L}{2} \right)^2 \right) \right\} L$$

(E.7)

**Note:** Two different cases are to be considered here for the boundaries different from the regular boundaries completely inside the simulation box. These are the boundaries intersecting the simulation cell along box_x and Oy and the half boundaries lying along box_y and Ox.

1) Dissipation along a regular boundary intersecting the boundary of a simulation box, where total flux is zero:

![Figure E.1: A regular boundary intersecting the boundary of a simulation box.](image_url)
For the boundary the flux must be zero at vertex \( v_1 \). However, for this type of boundaries, a local system is chosen having the center in a point where \( v_1 \) is located. The flux along this GB is:

\[
\mathcal{J} = \int_0^s - [B_0 \mathbb{U}_o] ds
\]

where,

\[
[B_0] = \begin{bmatrix} -n_x & -n_y \\ n_x & n_y & -(s+1_1) & n_x & n_y & -(s+1_2) \end{bmatrix}
\]

\[
[U_o] = \begin{bmatrix} v_{x1} & v_{y1} & \omega_1 & v_{x2} & v_{y2} & \omega_2 \end{bmatrix}^T
\]

By integrating the expression for \( \mathcal{J} \)

\[ J = [B] [U] \]

Where, \( [B] = \begin{bmatrix} n_1s & n_2s & -(0.5s^2 + l_1s) & -n_1s & -n_2s & (0.5s^2 + l_2s) & 1 \end{bmatrix} \]

\[
[U] = \begin{bmatrix} v_{x1} & v_{y1} & \omega_1 & v_{x2} & v_{y2} & \omega_2 \end{bmatrix}^T
\]

{There is no \( J_o \) here}

When evaluating the dissipation term associated with this boundary:

\[
\frac{1}{2} \int_0^s J^2(s) ds = \frac{1}{2} [U K_{mod} \mathbb{U}]
\]

Matrix \( [K_{mod}] \) can be obtained from the expression of matrix \( [K] \) from Equation (A.23) with following modification:

\[
s'_{old} = \int_{s_o}^{s} \mathcal{J}^2 ds = \frac{2}{3} \mathcal{J}^3 = \frac{2}{3} \left( \frac{L_{GB}}{2} \right)^3 = \frac{L_{GB}^3}{12}
\]

\[
s'_{new} = \int_{0}^{L_{GB}} \mathcal{J}^2 ds = \frac{L_{GB}^3}{3}
\]

Thus,

\[
s'_{new} = \frac{s'_{old}}{2}
\]

So, it can be deduced that the same expression for the matrix \( [K] \) can be used, provided \( s' \) is replaced by \( s'/2 \).

2) Dissipation along a half boundary, along the simulation cell boundary:

Power dissipation along a boundary segment is given by:

\[
\int_{-\delta/2}^{+\delta/2} \frac{k T}{2D \delta \Omega} J \cdot J ds
\]

For half-boundary, \( \delta \to \delta/2 \), the dissipation term becomes:

\[
\int_{-\delta/2}^{+\delta/2} \frac{k T}{2D \delta \Omega} J \cdot J ds
\]

The extra factor of 2 modifies the expression for dissipation and consequently, the elements of matrix \( [K] \) for this type of boundary.
Appendix F: Updating the Microstructure

Updating of microstructure, as it evolves with time as a result of deformation can be done by establishing the time-step for integration and updating the vertices positions.

F.1 Time-Step for Integration

A variable time-step is generated to keep the strain increments $\Delta \varepsilon$ for each time-step roughly equal. Assuming that the external force is applied along the Oy direction and the y component of the velocity of the box side is moving with $v_y$:

\[
\Delta L_y = v_y \Delta t
\]

\[
\Delta t = \frac{\Delta L_y}{v_y} = \frac{\Delta L}{L} \frac{L_y}{v_y}
\]

\[
\Delta t = \Delta \varepsilon \left( \frac{L_y}{v_y} \right)
\]

Thus, the generalized expression for time-step is:

\[
\Delta t = \Delta \varepsilon \left( \frac{L}{v} \right)
\]

where, L – Size of simulation box along the direction of traction.

$\sigma$ – Velocity of the edge along the direction of traction.

Figure F.1: Microstructure with simulation box dimensions and applied traction.
F.2 Updating the Vertices Positions

In Figure F.2, each of the three grains neighboring the vertex $v_0$ has three degrees of freedom and with the evolving structure; the GBs common with this vertex change their positions. For each grain, the position of the two boundaries containing $v_0$, can be evaluated after a short time interval $\Delta t$. The initial positions of all the vertices and GBs in the microstructure and the identity of each GB and its connected vertices should be noted and stored.

![Microstructure showing the vertex $v_0$ and its neighboring grains and vertices.](image)

**Method:**

For a given vertex $v_0$, identify the three GBs around it and label them as $gb_1$, $gb_2$ and $gb_3$. Now, given the position of the boundary $gb_i$, which is determined by the two vertices $v_0$ and $v_i$ at time $t$, we have to find the next boundary position at time $t+\Delta t$.

1) Identify the two cells bordering the GB.

2) Assume that the grain boundary $i$, i.e. $gb_i$, belongs to each of the two grains. Now, find the new position of ‘two’ new boundaries after time $\Delta t$.

3) Now, instead of the original $gb_i$, we have two new boundaries $gb'_i$ and $gb''_i$, represented by two lines. We know the equations of these two lines in our coordinate system. Hence, we can find out the equation of straight line bisecting the angles formed by these two lines. This equation, bisecting the smaller angle will represent the new boundary position for $gb_i$. (Figure F.3)
Figure F.3: New position of the gb\(_i\) after time \(\Delta t\) as angle-bisector of \(gb'\) and \(gb''\).

Equation of \(gb'\):
\[ x \cos \phi_1 + y \sin \phi_1 - p_1 = 0 \]

Equation of \(gb''\):
\[ x \cos \phi_2 + y \sin \phi_2 - p_2 = 0 \]

Here: \(\phi_1\) is the angle made by the normal to line \(gb'\) with the x-axis.
\(\phi_2\) is the angle made by the normal to line \(gb''\) with the x-axis.
\(p_1\) is the perpendicular distance of line \(gb'\) from the origin of axes.
\(p_2\) is the perpendicular distance of line \(gb''\) from the origin of axes.

Knowing the above two equations, the equation of a line bisecting the smaller angle formed by these two lines is given by:
\[ x(\cos \phi_1 + \cos \phi_2) + y(\sin \phi_1 + \sin \phi_2) - (p_1 + p_2) = 0 \]
Appendix G: Node Attraction

A virtual vertex attraction mechanism is implemented to enforce grain-switching events in a microstructure deforming by diffusional creep.

\[ V_e = \left| V_s \right| \times \left\{ \theta \left( \theta + \left( L_{gb} - L_{cr} / L_{cr} \right) \gamma \right) \right\} \]  

(G.1)

Where:

\[ | V_s | \] : Absolute value of the relative sliding velocity of the two neighboring grains bordering the grain boundary.

\[ L_{gb} \] : The actual length of the grain boundary.

\[ L_{cr} \] : The critical grain boundary length for neighbor switching.

\[ \theta, \gamma \] : Empirical constants (both positive) which control the contribution of the sliding velocity to the shortening of the grain boundary.

In our code, we may choose \( \theta = 10 \) and \( \gamma = 2 \) for our general microstructure.

\[ V_e \] : The relative velocity of the two vertices.

We may assume that both vertices move toward each other at the same velocity \( V_e / 2 \).

Figure G.1: Schematic representation of a GB and neighboring grains.
Given the characteristics of the microstructure, \( V_c \) can be calculated by using following method:

1. Calculate the relative sliding velocity

\[
\vec{V}_s = (\vec{V}_1 \cdot \hat{t} - \vec{V}_2 \cdot \hat{t}) \cdot \hat{t}
\]  

\( \hat{t} \) : Tangent unit vector

\( \vec{V}_1, \vec{V}_2 \) : Velocities of the centers of mass of Grain 1 respective to Grain 2.

\[
|\vec{V}_s| = |(\vec{V}_1 - \vec{V}_2) \cdot \hat{t} |
\]

Knowing that the tangent unit vector is given by:

\[
\hat{t} = \left( \frac{r_2 - r_1}{L_{gb}} \right) = \left[ \frac{(x_2 - x_1)}{L_{gb}} \right] \hat{i} + \left[ \frac{(y_2 - y_1)}{L_{gb}} \right] \hat{j}
\]  

\( \hat{i}, \hat{j} \) : Basis vectors

where:

\[
\vec{r}_1 = x_1 \hat{i} + y_1 \hat{j}
\]

\[
\vec{r}_2 = x_2 \hat{i} + y_2 \hat{j}
\]

are the coordinates of the two vertices \( v_1 \) and \( v_2 \).

Using,

\[
\vec{V}_1 = V_{1x} \hat{i} + V_{1y} \hat{j}
\]

\[
\vec{V}_2 = V_{2x} \hat{i} + V_{2y} \hat{j}
\]

we obtain:

\[
|V_s| = \left| \left( V_{1x} - V_{2x} \right) \cdot \left( x_2 - x_1 \right) / L_{gb} + \left( V_{1y} - V_{2y} \right) \cdot \left( y_2 - y_1 \right) / L_{gb} \right|
\]

Thus, knowing \( |V_s| \), one can then calculate the attraction velocities of any two nodes in the system. As mentioned previously, we assume that each node moves with velocity \( V_c/2 \) towards each other.
2. Calculate the absolute values of velocities of nodes 1 and 2 based on their relative velocity $V_e$.

$$\vec{V}_1 = \frac{V_e}{2} \cdot \hat{i} = \frac{V_e}{2} \left[ \frac{(x_2 - x_1)}{L_{gb}} \right] \cdot \hat{i} + \frac{V_e}{2} \left[ \frac{(y_2 - y_1)}{L_{gb}} \right] \cdot \hat{j}$$

$$\vec{V}_2 = -\frac{V_e}{2} \cdot \hat{i} = -\frac{V_e}{2} \left[ \frac{(x_2 - x_1)}{L_{gb}} \right] \cdot \hat{i} - \frac{V_e}{2} \left[ \frac{(y_2 - y_1)}{L_{gb}} \right] \cdot \hat{j}$$

Using MATLAB generate the following graphs:

$$\frac{V_e}{|V_s|} = \theta \left[ \theta + \left( \frac{L_{gb}}{L_{cr}} - 1 \right)^2 \right]$$

for

\[
\begin{align*}
\theta &= 5 \\
\theta &= 10 \\
\theta &= 15
\end{align*}
\]

Figure G.2: Graph of velocity ratio vs. GB length ratio.
VITA

Kanishk Rastogi belongs to the city of Jaipur, India. He finished his high school education in first class with distinction from Kendriya Vidyalava No.3, Jaipur, in 1997. Being always curious by nature and motivated by ‘how’ and ‘why’ behind everything, he decided to pursue a career in engineering. Kanishk joined Punjab Engineering College (PEC), Chandigarh, in year 1998 after going through a national level entrance exam and graduated with a Bachelor of Engineering in Metallurgical Engineering in year 2002. He then worked as Engineer (Inspection & Quality Assurance) in DCM Engineering Products (foundry), to gain a hands-on experience in problem-solving in a metallurgical environment.

Motivated by his passion for advanced studies, he joined Louisiana State University in Fall 2003 for his master’s in mechanical engineering, majoring in materials. He worked under the close supervision of his advisor Dr. Dorel Moldovan in the demanding field of materials modeling and simulation which is a fusion of metallurgical engineering, science and computation. His poster based on his research work was adjudged best in the 4th Annual Graduate Student Research Conference at Mechanical Engineering department in LSU. After his master’s program, he plans to work in a core materials engineering environment where he can put to use what he has learned so far.