PHASE FIELD SIMULATION OF GRAIN GROWTH IN PRESENCE OF SECOND PHASE PARTICLES

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Dedicated to my father

Shri Suresh Chandra Mallick
PREFACE

The dissertation entitled ‘Phase field simulation of grain growth in presence of second phase particles’ is submitted in partial fulfillment of the requirements for the award of the degree of Doctor of Philosophy in Mechanical Engineering at the National University of Singapore. The research described herein was conducted under the supervision of Dr. Srikanth Vedantam (Asst. Professor, Mechanical Engineering Department, NUS) and Prof. Lu. Li (Mechanical Engineering Department, NUS).

To the best of my knowledge, this work is original, except where acknowledgements and references are made to previous work. In my opinion, the work presented in this dissertation has reached the requisite standard fulfilling the requirement of Doctor of Philosophy. The result contained in this dissertation have not been submitted in part or in full, to any other university or Institute for the award of any degree, diploma or other qualification.

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ABSTRACT

Prediction of nucleation, grain growth, and concomitant microstructure in polycrystalline materials is of great technological importance because the size, shape, and the orientation of grains have a significant effect on the mechanical properties of materials.

In this thesis we first examine the effect of grain size - ranging from nano to micron sizes - on the elevated temperature tensile behaviour of a Magnesium alloy. We find a strong dependence of the tensile behaviour on the microstructure. Various characterisation techniques indicate the presence of particles and voids in the alloys which also affects the eventual microstructure formed. The control of microstructure, especially for nanocrystalline materials, has been recognized to be important in high temperature applications. In the remaining work we focus on the effect of second phase particles on the evolution of grains in such polycrystalline materials using a phase field theory. The connection of the microstructure formed to the mechanical properties is the scope of future work in this area.

We first construct a theoretical framework for the interaction of mobile second phase particles on a grain boundary. Since the time of Zener, most studies have focused on grain boundary interaction with immobile particles. However, many inclusions, voids and other defects may in fact be mobile and their interaction with grain boundaries is significantly different from immobile particles. Our theoretical study is restricted to the interaction of a single columnar grain with uniformly distributed particles and highlights many of the phenomena of grain boundary interaction with mobile particles.

For more realistic polycrystalline grain growth in the presence of mobile particles, we resort to a computational approach. Recently, phase field theories are becoming
popular for numerical simulation of grain growth. The phase field approach has developed for immobile particles and their effect on grain growth. In this thesis we develop this theory for the interaction of mobile particles and grain boundaries and we study the effects of this interaction in detail.

The mechanical properties of Mg-3%Al alloys are strongly dependent on the grain size, test temperature and the presence of second phase particles. Theoretical calculation for the interaction of columnar grain boundary and uniformly distributed mobile particles shows that the presence of particles has a strong effect on the grain boundary motion. If the particle mobility is higher than that of the mobility of the grain boundary, the particle will move along with the grain boundary. However, for low particle mobility, the grain boundary will have the tendency to detach from the particle which also depends on the curvature of the grain boundary. We calculate the transition radius for the different mechanisms of grain boundary motion. Our phase field simulation for bicrystal grain growth in presence of particles shows the effect of size and the mobility of particle on the kinetics of grain boundary. The mobile particles are dragged by the grain boundary and create a particle free band very similar to the experimental observation of Ashby and Gentamore (Acta Metallurgica (1968) 16, 1081).

Next we perform polycrystalline simulations using the phase field method. In polycrystalline particle-free simulations with grain boundary energy anisotropy, we observe that grain boundary energy anisotropy has a strong effect on the grain growth, grain size distribution and microstructural entropy. In a polycrystalline system with particles, the grain growth is retarded due to the presence of particles. The rate of retardation is higher when the particles are immobile than for mobile particles for the
same volume fraction and particle size. The average grain size as function of simulation
time depends on the size, volume fraction, and mobility of the particles present.
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NOMENCLATURE

\( \eta_i \) \hspace{1cm} \text{order parameter or phase field variable}

\( F \) \hspace{1cm} \text{total free energy}

\( f \) \hspace{1cm} \text{local free energy density}

\( f_m \) \hspace{1cm} \text{free energy density inside of grain matrix}

\( f_p \) \hspace{1cm} \text{free energy density inside of particle}

\( \alpha, \beta, \nu, \varepsilon \) \hspace{1cm} \text{coefficients of the local free energy density}

\( k_i \) \hspace{1cm} \text{gradient energy coefficient}

\( \kappa \) \hspace{1cm} \text{local curvature of the grain boundary}

\( \Delta \theta \) \hspace{1cm} \text{misorientation between adjacent grains}

\( \tau \) \hspace{1cm} \text{grain boundary thickness}

\( \varphi \) \hspace{1cm} \text{scalar function of order parameters}

\( Q \) \hspace{1cm} \text{total number of field variables or orientations}

\( Q_a \) \hspace{1cm} \text{total number of active parameters}

\( \delta \) \hspace{1cm} \text{the variational derivative}

\( \Delta f \) \hspace{1cm} \text{barrier height between the wells}

\( E_{gb} \) \hspace{1cm} \text{grain boundary energy}

\( a \) \hspace{1cm} \text{a constant for extended Read-Shockley grain boundary energy}

\( R_{ave}, D_{ave}, A_{ave} \) \hspace{1cm} \text{average radius, average diameter, average area of grain}

\( m \) \hspace{1cm} \text{growth exponent}

\( \alpha_i \) \hspace{1cm} \text{growth rate constant}

\( (\cdot)_t, (\cdot)_0 \) \hspace{1cm} \text{value at } t\text{-th step, initial value}
$S$  
microstructural entropy

$v$  
velocity of the grain boundary

$m_b$  
grain boundary mobility

$F_b$  
curvature dependent local driving force

$c$  
geometrical constant of grain

$\gamma_b$  
grain boundary energy per unit area

$\gamma_{bp}$  
local value of grain boundary energy

$R_o$  
initial grain radius

$R(t)$  
grain radius at time $t$

$\bar{R}, \bar{A}$  
nondimensional radius of grain, nondimensional area of grain

$\bar{R}_T$  
transition radius of grain

$\bar{R}_s$  
the critical radius at which particles are shed by the grain boundary

$v_p$  
velocity of mobile particle

$m_p$  
mobility of the particle

$F_p$  
local driving force on the particle exerted by the grain boundary

$V$  
Volume occupied by each particle

$f_v$  
volume fraction of the particles

$f_a$  
area fraction of the particles

$\gamma'_b$  

effective grain boundary energy in presence of mobile particles

$\nu_b$  
grain boundary velocity in presence of particles

$\nu (= m_p/m_b)$  
the ratio of particle mobility to grain boundary mobility

$\zeta$  
geometrical constant of the intersecting area of particle on grain boundary
\( E(t) \) total energy of grain boundary loaded with particles at radius \( R(t) \)

\( P_{gg} \) driving force for the particle free grain growth

\( P_{drag} \) pinning force by a single static particle

\( P_Z \) total pinning force per unit area of grain boundary

\( M \) particle mobility coefficient

\( p \) total number of particles

\( \theta \) boundary bypass angle

\( \bar{r} \) position vector of particle

\( R_Z \) limiting grain size

\( n \) number of particles per unit volume

\( n_s \) number of particles per unit area

\( D_{vol} \) diffusion coefficient

\( k_B \) Boltzmann constant

\( T \) absolute temperature in Kelvin

\( \mathbf{n} \) unit normal to the grain boundary

\( \mathbf{n}_{ij} \) unit vector in the direction of line joining the centers of the particles

\( \mathbf{f}_{ij} \) repulsive force between particles \( i \) and \( j \)

\( t \) grain growth time

\( \chi, b \) parameters for limiting grain size due to particle pinning
CHAPTER – 1

Introduction

The effect of microstructure on the mechanical behavior of materials has been well studied over the past several decades. In particular, the effect of grain size on mechanical properties has been extensively documented in several metals and alloy systems. For this reason, the control of grain size remains an important goal for material scientists and materials designers. Hence, a significant challenge for researchers in the material science community is to evaluate with grain morphology: grain size, grain boundary misorientation, recovery and recrystallization and kinetics and their influence with an aim to suggest optimal microstructure. One important mechanism which will be the focus of our work is the presence of second phase particles in metals and alloys and their effect on grain size and hence the physical properties of the metals.

Microstructure is the general term which concerns the microscopic description of small length scale constituents of materials, these include: precipitates, secondary phases, crystal structure (twins), grain size, orientation of grains etc. To understand and achieve optimum microstructure, there is a need to predict the temporal evolution of microstructure. Several theoretical, experimental and computational efforts have been made towards understanding microstructure evolution and its effect on mechanical properties. Some of them are reviewed in references [1-9] and more recent developments in [10-12].

There have been several studies of grain growth for single-phase alloy systems using Monte Carlo Simulation (MCS). The simulations are based on the calculation of the free
energy at each grid point in the lattice and compared to the value for a different random orientation. The new orientation is taken to replace the older one when the resulting free energy becomes lower or equal to the initial value. Other studies [13] have described a Q-state model using a variation of the MCS algorithm for grain growth in a polycrystalline material during sintering. The algorithm was developed for monophase or twophase structures considering both the square and triangular distribution of lattice points.

Cellular automata models for the kinetics of grain evolution have also been developed [14]. The continuous tracking of grain boundary and the curvature was estimated precisely. The simulation domain was divided into regular, square cells, where each cell represents a definite space in the material. The cells have two different possible states: one in which the cell is associated with a uniform property and a fixed crystallographic orientation representing the portion of the grain matrix. The other state is the grain boundary having fraction of two neighbouring grains with two different crystallographic orientations. The motion of the grain boundary depends on the driving force acting on the grain boundary, as given by Weygand et al. [15].

Lee introduced the Voronoi discretization method [16] for mesh free modeling of grain growth with the treatment of interface jump conditions. A new Voronoi diagram is obtained when an evolution point is inserted into a set of nodes. At every grain interior point, the material velocity was approximated by the non-Sibsonian shape functions, while slandered finite element shape functions were employed for the grain boundary velocity.

In addition to the methods listed above, the phase field method has proved particularly successful in describing microstructure evolution by computational
implementation. In phase field approach, no boundary conditions are required explicitly at the moving interface at each time step. The different phases in the material are represented by means of scalar field variables called the phase field variables and the phase boundary usually has small but finite thickness. Cahn and Hilliard [17] and then Allen and Cahn [18] were the first to develop the phase field theory in the context of curvature driven grain boundary motion. While the Cahn-Hilliard theory concerned the process of phase separation described by the conserved field variable, such as concentration, separating two domains of binary fluid, the Allen-Cahn theory studied non-conserved order parameters. The phase field method has been extensively used to numerically study microstructural evolution in multiphase systems, such as polycrystalline grain growth, solid-state phase transformations and martensitic transformations [19-22]. Recently the phase field models have also been efficiently applied in fracture mechanics [23], dislocation dynamics [24, 25], fluid mechanics [26, 27], wetting [28] etc.

In the phase field method as applied to polycrystalline grain growth, a large number of order parameters or field variables are employed. Chen and his co-workers [29-31] performed the phase field simulation for grain growth considering isotropic grain boundary energy while the effect of grain boundary energy anisotropy and mobility on grain growth was investigated by Kazaryan [32-34], Suwa [35, 36], Ko [37] among others. However, the main drawback in their simulations is the restriction of the number of order parameters to avoid the computational expense. As a consequence the anisotropic studies were restricted to low angle grain boundaries. In our approach, we used the active parameter tracking (APT) algorithm recently proposed by Vedantam and
Patnaik [38] to overcome the computational restriction on the number of order parameters allowed. We are thus able to investigate the effect of high-angle grain boundary energy anisotropy on grain growth.

Very recently, Moelans et.al [39, 40] proposed a phase field model for grain growth in the presence of finely dispersed immobile second phase particles. Suwa et.al [41] extended the same model to three dimensions. However, while there is experimental evidence to indicate that second phase particles may indeed be mobile [42-45], there have been no phase field models for grain growth in presence of dispersed mobile second phase particles.

The purpose of the research described in this thesis is to develop a theoretical and computational model for grain growth and its control by the presence of mobile and immobile particles. We use the multiphase field approach for simulation of microstructural evolution.

It is well understood that the growth process is more pronounced in smaller grains than in larger grains. In normal grain growth, the driving force for the grain boundary motion is proportional to the local curvature (curvature $\kappa = 1/R$, where $R$ is the radius of curvature) of the grain boundary. Thus normal grain growth primarily depends on the curvature of the grain boundary.

In Chapter 2, we begin with an experimental investigation of the effect of grain size on the mechanical properties. In our experiments we study nanocrystalline, ultrafine and microcrystalline size grained bulk samples and their temperature dependent mechanical properties. In the small grain sized samples, the grain growth is expected to be very rapid in single-phase alloys at elevated temperatures due to grain boundary motion without
obstacles. However in the Mg-Al alloys tested, grain growth even in the smallest grain size samples is found to be minimal [46]. Presumably this is because finely dispersed second phase particles present in these alloys control the grain growth and thus improve the mechanical properties. In Mg-Al alloys, the presence of second phase particle has been found to be very effective in inhibiting grain growth at higher temperature [47-49].

We next focus on the mechanism of grain growth inhibition by second phase particles. In chapter 3, we develop a mathematical model of grain growth in presence of second phase mobile particles. A single columnar grain with randomly distributed spherical particles is considered. The second phase particles are given a simple constitutive relation by which the particle velocity is proportional to the driving force arising from the curvature of the phase boundary. We show that the grain boundary kinetics depends on particle mobility and the volume fraction of particles present.

In chapter 4, we study the interaction of a bicrystal grain boundary with a single particle in two dimensions. We consider a system of a radially symmetric grain boundary consisting a circular shrinking grain embedded by another grain. Initially the particle is located inside of the circular grain. We develop and use a phase field model for this purpose. A specific form of free-energy common to all phase field theories and appropriate evolution laws for the order parameters are used in this model. The growth rate of the circular grain depends on the size of the particles present as well as the coefficient of the mobility of the particle.

In chapter 5, the effect of energy anisotropy in the grain growth process for a single-phase polycrystalline material is modeled using the phase field approach. In this extended phase field model, the energy anisotropy is not restricted to low angle misorientations
between adjacent grains as in previous studies. The high angle grain boundary energy is taken to be given by an extension of Read-Shockley energy for low angle grain boundary [50]. It is observed that the extended Read-Shockley energy system has significantly lower grain growth rate, followed by Read-Shockley and isotropic grain boundary energy.

Chapter 6 deals with the phase field simulation for microstructural evolution in a polycrystalline crystalline system in the presence of monodisperse second phase mobile and immobile particles. Initially particles are randomly distributed over the volume of the material in two dimensional setting. The presence of particles significantly retards the grain growth process. The microstructure becomes effectively pinned in presence of immobile particles while the presence of mobile particles allows the motion of grain boundaries at effectively slower rates. The growth rate is approximated by a power law, 

\[ \langle R(t) \rangle^m - \langle R_0 \rangle^m = \alpha_1 t \]

with the exponent \( m > 2.0 \). The value of \( m \) is found to increase with the increasing volume fraction of particles.

Finally the conclusions and possible extensions in future work are summarized in chapter 7. The connection of the microstructure to the mechanical properties remains a subject for future work. Furthermore, the implementation of particle evolution is an important step towards realistic simulation on grain growth in bulk polycrystalline materials. Sub-grain coalescence via grain rotation for nanocrystalline materials may be a major extension of the present simulation work. The phase field model has the advantage of being amenable to such an extension.
CHAPTER – 2

Experimental studies of grain size dependent mechanical properties of Mg-3%Al alloy at elevated temperatures

2.1 Introduction

Many of the mechanical properties of bulk crystalline materials, such as yield strength, ultimate tensile strength, hardness, the ductile-brittle transition temperature and super-plasticity depend on the grain size of a material and can be improved by refining the grain size [51, 52]. The main goal of the material scientist is to develop new engineering materials with superior properties. With this goal, researchers are working towards controlling grain growth by inclusion of second phase particles. It is well known that the reduction of grain size gives better strength (Hall-Petch relation). However, the main drawback of very small grain sized materials (such as nanocrystalline material) is that they are relatively thermally unstable and very sensitive to small increase in temperatures [53]. The grain boundary recovery time is inversely proportional to the size of grain and thus faster structural transformation have been found to occur in nanosized grains [54]. Moreover, nanocrystalline materials have some special mechanisms for the kinetics of grain boundary such as rotation of grains and lower trigger temperature for grain growth [55]. As a result, in these materials, higher grain growth rate is observed than in coarse grained polycrystalline material [56]. Thus, the choice of nanocrystalline and ultrafine material for experimental investigation of grain size dependent mechanical properties at elevated temperatures in the context of the study of grain growth is
important. In this chapter, we experimentally investigate grain size dependent mechanical
properties of Mg-3\%Al alloy at different temperatures.

Bulk nanostructured Mg-3\%Al alloys were prepared by mechanical alloying and the
microstructure and mechanical properties were characterized. Tensile tests were
performed at elevated temperatures up to 250\textdegree{}C and the yield strength, tensile strength
and elongation to failure were measured for microcrystalline (14 \(\mu\)m) and nanocrystalline
(120 nm and 90 nm) samples. Remarkably, the strain to failure was observed to be non-
monotonic with temperature with the failure strain increasing up to a critical temperature
and decreasing thereafter. This critical temperature was found to be strongly dependent
on grain size. This phenomenon is attributed to a competition between uniform
elongation and necking deformation. The latter dominates at higher temperatures due to
decreased strain hardening, particularly in the fine grained samples.

2.2 Magnesium and its alloy

Magnesium and its alloys are being studied intensively because of their potential
applications in the automotive and aerospace industries, where weight savings and
resulting increase in fuel efficiency are very important. Magnesium is the one of the
lightest (density~1.74 gm/cm\(^3\)) and abundant metallic materials with excellent
mechanical properties such as machinability, castability, thermal conductivity,
weldability, creep resistance, strength/weight ratio, and damping capacity. However, its
low strength, low ductility and poor corrosion resistance compared to aluminum, have led
researchers consider its alloys [57-61] for applications.
Furthermore, fine grained Mg alloys have been found to have superior properties, particularly strength, compared to coarse grained Mg alloys in accord with the Hall-Petch relationship. The most widely used techniques for the synthesis of fine grained Mg alloys are either through severe plastic deformation, such as high pressure torsion, equal channel angular pressing, accumulative roll-bonding[62-65] or powder metallurgy techniques such as consolidation of mechanically milled powders [60, 66]. In this work, we use the latter technique to obtain and study nanocrystalline (NC) and microcrystalline (MC) samples. Many of the applications of these alloys require operation at elevated temperatures of up to 250°C [67, 68]. There have only been a few studies of the mechanical properties of Mg-Al alloys at elevated temperatures so far. In this work we experimentally study the tensile behavior of nanocrystalline (NC) Mg-3%Al alloy at test temperatures ranging from room temperature to 250°C. The properties are compared with those of a microcrystalline (MC) counterpart. These observations are expected to have important consequences for applications and processing of these materials.

2.3 Experimental procedures

Commercial elemental powders of Mg and Al with purity of 99.5% were mixed at the weight ratio of 97:3 Mg to Al. To prevent agglomeration and excessive cold welding of the powders, 1.4 to 2.2 wt% stearic acid was added. Nanostructured powder of Mg-3% Al alloy were obtained by ball milling of the powder in an inert atmosphere. The duration of the milling was either 20 hours or 30 hours to obtain different particle sizes. The milled powders were than packed in a die and sealed by grease to prevent oxidation inside of the glove box as shown in figure (2.1). The consolidation of the mechanically
alloyed powders was carried out by cold compaction followed by sintering at 450°C for 2 hours in an Argon furnace. A 7 mm diameter rod was extruded from the sintered compact. The hot extrusion was performed at 350°C with an extrusion ratio of 25:1. Further details pertaining to the processing technique have been presented in [60]. Microcrystalline (MC) rods were obtained from processing unmilled powders whereas two different nanocrystalline (NC20 and NC30) rods were obtained from processing the powders milled to 20 hours and 30 hours respectively.

Figure 2.1: Schematic representation of consolidation of nanocrystalline ball milled powder by applying an isostatic pressure.

X-ray diffraction (XRD) analysis was carried out to analyze the structure of mechanically alloyed powder and the bulk samples using a Shimadzu Lab XRD-6000 X-ray diffractometer with CuKα diffraction at wavelength of, λ =1.54056 Å. The operating voltage of the diffractometer was 40kV an anode current of 30mA. The grain size of nanocrystalline samples was calculated using Hall-Williamson method. High-resolution optical microscope was used to calculate the grain size of microcrystalline samples. Field
emission scanning electron microscope (FESEM) was employed to examine the fracture surface of tensile specimens and the microstructure of etched samples.

Round cross-sectioned specimens with gauge diameter of 5mm and 25mm gauge length were machined from the extruded rod in accordance with the ASTM E8M-96 standard. Tests were performed on an Instron-8874 machine at temperatures ranging from room temperature to 250°C in air. An initial strain rate \(4 \times 10^{-4} \text{s}^{-1}\) was employed at all test temperatures. Specimens were soaked for 20 min at the designated temperature prior to test to obtain thermal equilibrium. Tensile properties were estimated based on the average of three tests for each test condition.

2.4 Results and discussion

2.4.1 Crystallographic representation and grain size calculation

The crystallographic structure of the MC and NC\textsubscript{20} and NC\textsubscript{30} samples were analyzed by X-ray diffraction peak profile. Figure 2.2 shows the XRD spectra of Mg-3%Al alloy powder and extruded rods of the unmilled and milled samples. It was observed that \(\alpha\)-Mg is the dominant phase for all XRD spectrums. In figure 2.2(a), the diffraction peaks of Al (1 1 1) are clearly noticed only in the unmilled powder sample but not in other mechanically milled samples. After mechanical alloying, the Al peak disappears and peaks corresponding to minor phases of Mg\textsubscript{17}Al\textsubscript{12} appear, as indicated by the (3 3 0) and (3 3 2) peaks. The decrease of the intensity of Bragg peaks and the increase of full width at half maximum (FWHM) at the same position with the increase of milling hours indicating that a reduction in the grain size has taken place and that lattice strain was introduced by the mechanical milling.
Figure 2.2(b) shows the diffraction spectra of the extruded rod. The lower intensity of Mg (0 0 2) peak indicates that the basal plane rotates preferentially in the direction of [1 0 1] to coincide with the extrusion direction. Nevertheless, the intensity of (1 0 0), (1 1 0) and (2 0 1) diffraction peaks of Mg were increased indicating the formation of textured structure. The Mg$_{17}$Al$_{12}$ peak was observed in the unmilled sample, whereas in the milled samples this peak disappears after sintering, consistent with [69]. The peaks of MgAl$_2$O$_4$ were intensified in milled samples indicating that the formations of oxide particles are proportional with milling duration. The FESEM image of extruded sample as shown in the figure 2.3 confirms the presence of precipitated second phase Mg$_{17}$Al$_{12}$ particles which is present in the unmilled bulk sample.
The grain sizes of the samples were calculated by Hall-Williamson method. The grain sizes of the powdered milled samples were obtained to be ~40 nm and ~30 nm for the NC$_{20}$ and NC$_{30}$ samples respectively. After sintering the grain sizes were estimated to be ~120 nm for the NC$_{20}$ samples and ~90 nm for the NC$_{30}$ samples, consistent with the estimates in [69]. The grain size in the MC samples was measured about 12 µm optically. The grain size also estimated after the tensile tests at all temperatures were performed and did not indicate any significant grain growth.

2.4.2 Tensile properties

Figures 2.4, 2.5 and 2.6 show the engineering stress-strain curves at different temperatures for the MC, NC$_{20}$ and NC$_{30}$ samples, respectively. All three samples show brief work hardening followed by a continuous stress drop to failure at all temperatures. The yield strength, ultimate tensile strength and strain hardening decrease with temperature for all the samples.
Figure 2.4: Engineering stress-strain curves for the MC samples at different temperatures.

Figure 2.5: Engineering stress-strain curves for the NC$_{20}$ samples at different temperatures.
Figure 2.7: Variation of the yield strength (Y.S) and ultimate tensile strength (U.T.S) as a function of test temperatures.

Figure 2.6: Engineering stress-strain curves for the NC\textsubscript{30} samples at different temperatures.
Figure 2.7 shows the variation of the yield strength and ultimate strength with temperature. The data points represent the average of four tests and the standard error of the mean is represented as error bars in the figure. The yield strength of the NC samples is higher than that of the MC sample at room temperature but drops more rapidly with temperature. The rapid decrease in strength with the increase in temperature is caused by the activation of grain boundary sliding. Since the NC samples have higher grain boundary area per unit volume relative to the microcrystalline samples, at low temperatures the grain boundaries act as obstacles to the migration of dislocations and twinning, if any. At higher temperatures, the grain boundaries are thermally activated and lead to thermally assisted sliding [70].

![Graph showing the variation of failure strain with test temperature](image_url)

Figure 2.8: Variation of the failure strain ($\varepsilon_t$) as a function of test temperatures.
Figure 2.8 shows the variation of the failure strain ($\varepsilon_f$) of the three samples at the different temperatures. It can be noted that the failure strain is nonmonotonic and the maximum occurs at lower temperature for the smaller grain sized samples. This is due to the strong dependence of the work hardening with temperature for samples of all three grain sizes. This, in conjunction with the decrease in yield stress, results in a drop in the ultimate tensile strength (UTS) with temperature for samples of all grain sizes. The effect of the decrease in work hardening is most significant on the strain to failure in the three specimens.

The failure strain is dependent on the competition between uniform deformation and necking as seen in the photographs shown in figure 2.9. It can be seen that the onset of necking occurs at a much lower temperature in the NC$_{30}$ samples in figure 9(ii) than the MC samples in figure 9(i). Grain boundary deformation processes, e.g. grain boundary diffusion creep, interfacial sliding, and grain boundary shear led to improve in ductility for NC samples at room temperature. However, due to the lower strain hardening present at higher temperatures, necking is more pronounced and the failure strain drops. The loss of strain hardening is due to the decreased pile-up of dislocations at higher temperature. This effect is strongly dependent on the grain size and the rapid lowering of strain hardening with temperature for the finer grain specimens promotes necking at lower temperatures. This results in the non-monotonic dependence of the failure strain on temperature. For the MC samples, the failure strain increases up to 150$^\circ$C. However, in the NC$_{20}$, the failure strain increase up to 50$^\circ$C above which it decreases. In the NC$_{30}$, the failure strain decreases above room temperature. Presumably, the peak failure strain
occurs at or below room temperature for the NC\textsubscript{30} sample. These observations are confirmed by the necking observed in the tensile samples shown in figure 2.9.

![Figure 2.9: Photographs of the (i) unmilled and (ii) 30 hrs milled tested samples. For the unmilled samples, the tests were performed at (a) RT (b) 50\textdegree C (c) 100\textdegree C (d) 150\textdegree C (e) 200\textdegree C and (f) 250\textdegree C. The 30 hrs milled samples were tested at (a) RT (b) 50\textdegree C (c) 100\textdegree C (d) 150\textdegree C (e) 250\textdegree C. An untested sample of each is shown below for reference.](image)

2.4.3 Fracture properties

Figures 2.10 and 2.11 show the fracture surfaces of tensile specimens tested at room temperature and 250\textdegree C respectively. A very rough surface (due to larger grain size) with cleavage type fracture is observed in the MC sample (see figure 10(a)). Figure 2.10 (b) and figure 2.10(c) depict "grain like" shearing structures with finer structure on the fracture surface. Two distinct fracture modes can be identified from fracture morphology of the NC\textsubscript{20} and NC\textsubscript{30} samples when compared to the coarse-grained counterpart. In the NC samples, the fine grain size presents an intergranular mode while the fracture morphology of the coarse-grained sample gives transgranular cleavage mode. The fracture morphology of tensile specimen tested at 250\textdegree C is significantly different from that of room temperature as shown in figure 2.11. The area fractions of microvoids as
well as cluster of grains are also higher in the NC samples as seen in figure 2.11(b) and figure 2.11(c) which also contribute to the low fracture strain. The fracture surface morphology is in accord with the fracture strain obtained in the tensile tests. A similar observation was recorded in cryomilled ultrafine Al-7.5% Mg alloy deformed at temperatures in the range 100–300°C[70].

2.5 Conclusions

In conclusion, microcrystalline and two different grain sized nanocrystalline samples of Mg-3%Al alloy were obtained by a ball milling process for different durations. The
extruded samples were characterized by XRD, FESEM and optical microscopy. Tensile tests were performed at elevated temperatures up to 250°C. The tensile properties were found to be strongly dependent on the grain size and temperature. In particular, the strain hardening decreased rapidly with temperature especially in the finer grained specimens causing significant necking at lower temperatures for the NC samples. The loss of strain hardening and thus the reduction of strength is the result of the decreased pile-up of dislocations at a higher temperature. Domination of necking over uniform elongation resulted in a non-monotonic failure strain. The peak failure strain occurred at lower temperatures in the NC samples. These observations are expected to have important consequences in the processing and application of these technologically useful alloys.
CHAPTER – 3

Theory of grain growth in presence of second phase mobile particles

3.1 Introduction

In this chapter, we study the effect of mobile second phase particles on grain growth. Grain growth is generally controlled by the presence of immobile particles through the pinning of grain boundary. However, there are some cases where second phase particles are mobile and can be dragged by the grain boundaries [42, 43, 45] or other mobile interface [71]. This mobile nature of particles is commonly observed in sintered material. In this chapter, we are interested in developing a theoretical analysis for grain boundary migration in presence of second phase mobile particles.

In order to develop an analytical framework, we consider the evolution of a single columnar grain in the presence of randomly distributed second phase particles. We study the evolution of the grain under the constitutive assumption that the particle velocity is proportional to the driving force of the grain boundary. This model provides physical insight into the conditions for grain boundary arrest by, or detachment from, the particles.

The particle can be defined as mobile if the particle has capability to move with the grain boundary. The rate of movement of the particle depends on its mobility and the driving force (proportional to the curvature of grain boundary) exerted by the grain boundary where that particle is located. The mobility of these particles is inversely proportional to the third or fourth power of the particle radius (depending on the atomic transport mechanism [72]) and may be quite significant in dispersions of fine particles.
Thus an assumption that the particles are immobile in these cases would not be realistic. There have been a few recent theoretical and numerical studies of the effect of mobile particles on grain growth. The theoretical studies on shape change of bicrystal half-loops [72] and quarter-loops [73] and numerical studies using Monte Carlo simulations [74], cellular automata [71] and statistical methods [75, 76] have shed important light on the growth rates in the presence of mobile particles.

The main purpose of this chapter is to focus on a circular shrinking grain and study the conditions under which the grain boundary drags the particles or detaches from them. We present our calculations in single columnar grain in a matrix; extension to the case of a spherical grain in a matrix poses no conceptual difficulties.

3.2 Theory of grain growth

Let us consider a columnar grain of circular cross-section and length $L$ in a matrix in which spherical mobile second phase particles are uniformly dispersed as shown in Figure 3.1.

![Figure 3.1: The schematic of the grain boundary sweeping mobile particles. (a) The columnar grain with circular cross-section embedded in a matrix with particles. (b) The cross sectional view of the columnar grain (a). The initial grain boundary is shown using a dotted line while the current location of the grain boundary is shown using the solid line. The swept region is devoid particles.](image-url)
In the absence of particles the circular grain minimizes its grain boundary energy by shrinking towards its center. The velocity of the circular grain boundary with out the presence of particle is given by

$$v = m_b F_b$$  \hspace{1cm} (3.1)

where \(v\) is the velocity of the grain boundary and \(m_b\) is the boundary mobility. \(F_b\) is the curvature dependent local driving force for which the grain boundary was shrinking towards the center of curvature of the circular grain. This force can be expressed as [77]

$$F_b = -c \kappa \gamma_b$$  \hspace{1cm} (3.2)

where \(c\) is the geometrical constant and its value is equal to one for a circular grain and two for spherical one. \(\gamma_b\) is the grain boundary energy while \(\kappa = 1/R\) represent the radius of curvature. Thus, for a circular grain equation (3.1) and (3.2) yield

$$v = \frac{dR}{dt} = -\frac{m_b \gamma_b}{R}$$  \hspace{1cm} (3.3)

Integrating equation (3.3) following nondimensional radius of the grain was obtained,

$$1 - \bar{R}^2 = \frac{2m_b \gamma_b}{R_o^2} t, \hspace{1cm} \text{with } \bar{R} = R(t)/R_o.$$  \hspace{1cm} (3.4)

In the above equation, \(R_o\) is the initial grain radius (at \(t = 0\)) while \(R(t)\) is the radius at time \(t\).

Now let us take \(n\) spherical particles of radius \(r_p\) per unit volume, with each particle occupying volume \(V\). Then the volume fraction (\(f_v\)) of the particles in the material is given by

$$f_v = nV.$$  \hspace{1cm} (3.5)
The following constitutive relation for the velocity of the mobile particle was assumed [72]
\[ v_p = m_p F_p, \]  
(3.6)
where \( m_p \) is the mobility of the particle and \( F_p \) is the local driving force on the particle exerted by the grain boundary. The mobility of particle \( m_p \) is inversely proportional to the particles radius as, \( m_p \sim \frac{1}{r_p^q} \) with \( q = 3 \) or \( 4 \) depending on the transport mechanism (e.g., bulk/interfacial diffusion in the matrix/particle) while the constitutive relation Eq. (3.6) remains unchanged for the different mechanisms. The particle mobility for various types of inclusions and atomic transport mechanisms is collated in [72]. The local driving force \( F_p \) is proportional to the local curvature of the grain boundary and for a circular grain, \( F_p = -\gamma_b \kappa \). Thus, the equation (3.6) for particle velocity yield,
\[ v_p = -m_p \gamma_b \kappa = -\nu m_b \gamma_b \kappa \]  
(3.7)
where, \( \nu = m_p / m_b \) is a constant term. Now the new form of constitutive relation for grain boundary velocity in presence of particles are obtained as follows:
\[ v_{bp} = -m_b \gamma'_b \kappa \quad \text{with} \quad \gamma'_b = (1 - \nu) \gamma_b. \]  
(3.8)
The \( \gamma'_b \) is an effective grain boundary energy in presence of mobile particles. The grain boundary energy changes with the grain radius since it picks up particles as it sweeps through the material. In general, the intersection of the particles with the grain boundary changes the local value of the grain boundary energy to \( \gamma_{bp} \). We will assume that \( \gamma_{bp} = 0 \).
Then the change in grain boundary energy for an incremental change in radius is given by

\[ d\gamma_b' = \left( \frac{\text{number of particles swept} \times \text{interaction area per particle}}{\text{area of grain boundary}} \right) \gamma_b'(R) \]

\[ = \frac{(n2\pi R dRL)\zeta\pi r_p^2}{2\pi RL} \gamma_b'(R) \]  

(3.9)

where \( n2\pi R dRL \) is the total number of particles picked up by the grain boundary as it sweeps an incremental volume \( dV = 2\pi R dRL \) and \( \zeta\pi r_p^2 \) is the area of cross section of each particle intersecting the grain boundary with \( \zeta \) being a geometrical constant representing the intersection of the particle with the grain boundary. The coefficient of \( \gamma_b' \) in Eq. (3.9) represents the fraction of area lost to particles.

Equation (3.9) can be integrated from an initial radius \( R_0 \) with grain boundary energy \( \gamma_{bo} \) to obtain the grain boundary energy as a function of radius \( R(t) \),

\[ \gamma_b' = \gamma_{bo} e^{-\xi(1-\bar{R})} \quad \text{with} \quad \xi = n\zeta\pi r_p^2 R_0. \]  

(3.10)

The term \( \bar{R} = R(t) / R_0 \) is the nondimensional radius. For the sake of convenience, we take \( \gamma_{bo} = \gamma_b \); that is, the grain boundary is particle free at \( R(0) = R_0 \).

Note that, for a columnar grain, the curvature \( \kappa = 1/R \) where \( R \) is the radius of the grain.

3.3 Illustrative case study

In this section, we present simple analytically tractable example which provide a first illustration of the theory of grain growth in presence of mobility dependent mobile
particles. In addition the analytical value of illustrative examples should also be useful for constructing numerical approximation to more complex system.

3.3.1 Case I: Particle mobility \( m_p \) > Grain boundary mobility \( m_b \)

If the particle mobility is greater than the grain boundary mobility then the velocity of the particles is limited by the grain boundary velocity. Such a case may occur for fine particles since the mobility is inversely proportional to the third or fourth power of the particle size depending on the mobility mechanism [72].

As the grain shrinks, it sweeps the particles in its path and they accumulate on the grain boundary. We show the two-dimensional cross section in Figure 3.1(b) (compare this schematic with the optical micrograph in Figure 2 of [43]). When the radius of the grain is \( R \) the velocity of the loaded grain boundary (from Eqs. (3.8) and (3.10)) is given by

\[
v_{b_p} = \frac{dR}{dt} = -m_b \gamma_{bo} e^{-\xi(1-\bar{R})} \kappa. \tag{3.11}
\]

The equation (3.11) can be expressed as,

\[
v_{b_p} = R_o \frac{d\bar{R}}{dt} = \frac{-m_b \gamma_{bo} e^{-\xi(1-\bar{R})}}{\bar{RR}_o}, \tag{3.12}
\]

where \( R(t) = \bar{RR}_o \) and the curvature \( \kappa = 1/\bar{RR}_o \). Integration of Eq. (3.12) yields,

\[
\frac{2}{\xi^2} \left( 1 + \xi \bar{R} \right) e^{\xi(1-\bar{R})} - (\xi + 1) = \frac{2m_b \gamma_{bo} \bar{R}}{R_o^2 t}.
\tag{3.13}
\]

We note that the left hand side of the above equation matches Eq. (3.4) for \( \xi \to 0 \). A plot of nondimensional radius (\( \bar{R} \)) from Eq. (3.13) for two values of \( \xi = n \pi \xi n_p^2 R_o \) is compared to particle free grain evolution given by Eq. (3.4) in Figure 3.2. The solid line represents
particle free evolution and Eq. (3.13) is shown for $\xi = 1$ (dashed line) and $\xi = 5$ (dash-dot line). It is seen that for a larger number of particles per unit area or larger particle radius (increasing $\xi$), the grain boundary motion is slower. From Eq. (3.13), it is seen that the grain boundary velocity is non-monotonic and the minimum velocity occurs at $\bar{R} = 1/\xi$.

Since the mobility of the particles is higher than that of the grain boundary, the grain boundary cannot detach (neither grain boundary move fast nor slow from the particle) from the particles in this case as the particle pushed only by the curvature driven grain boundary force.

![Figure 3.2: A plot of the radius of the circular grain vs non-dimensional $\tau = \left(2m_p\gamma_b/R_o^2\right)t$ for $m_p > m_b$. The solid line represents evolution in the absence of particles given by Eq. (3.4) and $R(t)$ from Eq. (3.13) for different $\xi = n\kappa\sigma_p^2R_o$ is shown using the dashed line ($\xi = 1$) and dash-dot line ($\xi = 5$).]
3.3.2 Case II: Grain boundary mobility ($m_b$) $>$ Particle mobility ($m_p$)

The particle velocity limits the grain boundary motion if the grain boundary mobility is greater than that of the particle mobility. The velocity of the grain boundary in the particle-limited case is given by

$$v_b = -m_p \gamma_b \kappa$$  \hspace{1cm} (3.14)

Alternatively, for a grain boundary loaded with particles, the driving force for the grain boundary is smaller (because of the energy reduction due to the particles) and hence its velocity is given by Eq. (3.12). The radius at which the grain boundary velocity transitions from particle limited case to grain boundary limited case is obtained by equating the grain boundary velocity ($v_b$) from Eq. (3.14) to that from Eq. (3.12). The transition radius is thus given by

$$R_T = \frac{1}{\xi} \log(m_p / m_b).$$  \hspace{1cm} (3.15)

It is seen from the above equation that if the number of particles per unit area $n$ or the particle radius is large, the transition radius is closer to $R_b$. On the other hand, if the particle mobility is small compared to the boundary mobility, then the transition from the particle limited motion to boundary limited motion occurs at smaller $R$.

The transition radius is shown in Figure 3.3 for $\xi = 2$ and $m_p/m_b = 0.6$. Above $R_T = 0.75$ the grain is limited by the particle mobility and below $R_T = 0.75$, the grain boundary driving force is lower due to the presence of the particles.

In the case of $m_p < m_b$, the grain boundary has the ability to free itself from the particles. This happens when the free energy change due the particle free boundary motion is greater than that due to particle loaded grain boundary motion.
3.4 Energy based calculation of critical radius for shedding of particle

In this section, we use an energy-based criterion to determine the critical radius of the grain boundary for particle shedding. The energy of the grain boundary loaded with particles at radius $R(t)$ is given by

$$E(t) = 2\pi R(t)\gamma_b^t(R(t)).$$  \hspace{1cm} (3.16)

The grain boundary has two choices at every instant of time. It can drag the particles along with it or snap through leaving them behind. Each of these choices allow the grain boundary to move by different velocities. We assume that the choice leading to smaller total energy for the system at time $t+\Delta t$ is chosen by the grain boundary. In the event that

![Figure 3.3: A plot of the radius of the circular grain vs non-dimensional radius $\bar{R}$ for $m_p/m_b = 0.6$ and $\xi = 2$. The dashed line represents particle limited evolution whereas the solid line shows the grain boundary (GB) limited evolution of the grain. The grain evolution transitions from the dashed line above $R_T$ to the solid line below $R_T.$]
the particles are shed by the grain boundary, the change in energy of the system is given by

\[ \Delta E_1 = 2\pi R_1(t+\Delta t)L\gamma_b - 2\pi R(t)L\gamma'_b(R(t)) \]  

(3.17)

where \( R_1(t+\Delta t) \) is the radius of the grain boundary at time \( t+\Delta t \) assuming that it moved with the particle free velocity \( v_b = -m_b\gamma_b / R \). On the other hand, if the grain boundary drag the particles, the energy is given by

\[ \Delta E_2 = \Delta t \frac{d}{dt}(2\pi R L\gamma'_b(R)). \]  

(3.18)

The choice of whether the boundary sheds the particles or drags them along depends on whether \( \Delta E_1 \) or \( \Delta E_2 \) is larger. Particles are shed if \( \Delta E_1 < \Delta E_2 \) and are dragged along if \( \Delta E_1 > \Delta E_2 \). This choice arises because the increase in the total energy due to shedding of the particles is compensated by the decrease in grain boundary energy due to faster particle free grain boundary motion. Since the grain boundary has to move a minimum distance of the size of the particle in order to shed the particles, we obtain \( \Delta t = \frac{\lambda r_p}{v_b} = \frac{\lambda r_p R}{m_b\gamma_b} \) where \( \lambda \in (0, 2) \) is a geometric parameter which depends on where the particle intersects the grain boundary. Note that the geometrical constant \( \zeta \) introduce in Eq. (3.9) is related to \( \lambda \) through: \( \zeta = 1 - |1-\lambda| \). Substituting \( R_1(t+\Delta t) = R(t) - m_b\gamma_b\Delta t/R(t) \) in Eq. (3.17), we solve the Eqs. (3.17) and (3.18) to obtain an implicit condition for the critical radius \( \bar{R}_s \) at which the particles are shed by the grain boundary

\[ \bar{R}_s - \frac{\lambda r_p}{R_0} - \bar{R}_s \exp(\xi(\bar{R}_s-1)) = -\frac{\lambda r_p}{R_0}(1 + \xi\bar{R}_s)\exp(2\xi(\bar{R}_s-1)). \]  

(3.19)
For large $\bar{R}$, $\Delta E_1 > \Delta E_2$ and it is energetically preferable for particles to be dragged long by the grain boundary. From Eq. (3.19), it can be seen that as $\xi \to \infty$, $\bar{R} \to \lambda r_p / R_o$. This implies that in the presence of a larger number of particles per unit volume or large particle radius, the transition from particle dragging to particle shedding occurs at $\bar{R} \approx \lambda r_p / R_o$.

3.5 Summary and concluding remarks

We have presented theoretical calculations describing the interaction of a columnar grain boundary and uniformly dispersed mobile particles in an axisymmetric setting. By assuming a constitutive relation for the velocity of the particles in terms of the driving force arising from the curvature of the grain boundary we derive conditions under which the grain boundary is slowed, arrested or detaches from the particles.

We find that:

1. For $m_p > m_b$: the grain boundary is slowed down and may become arrested due to the accumulation of particles on the grain boundary.

2. For $m_b > m_p$:
   
   (a) the grain boundary evolution begins as particle limited motion but transitions to grain boundary limited motion at the radius given by equation (3.15).
   
   (b) particles can be shed by the grain boundary at the radius given by equation (3.19). This happens when the decrease in energy due to faster movement of the boundary compensates for the increase in energy due to particle shedding.
In deriving the above conditions, we have assumed that the intersection of the particles with the grain boundary does not contribute to the interfacial energy. In reality, the grain boundary energy changes in the presence of the particles. While the calculations become algebraically more cumbersome, the main conclusions are unaffected. Our simulation result (discussed in the next chapter) using a phase field theory will also corroborate these conclusions.
CHAPTER – 4

Bicrystal model for grain growth containing mobile second phase particle: Phase field approach

4.1 Introduction

In this chapter, we develop a phase field model for grain growth in the presence of mobile second phase particles. In the model, each grain and particle is represented by a unique order parameter. We consider that the particle velocity to be proportional to the driving force arising from the curvature of the phase boundary in the neighbourhood of the particle. The proportionality factor is the constitutive parameter representing the mobility of the particle. We present the phase field model in a one-dimensional axisymmetric setting and compare with theoretical results. We then study the interaction of a bicrystal grain boundary with particles in the limits of dilute and dense distributions.

It is well known that the mobility of grain boundary plays the key role for the kinetic behavior of grain boundaries and hence the grain growth of materials. Most new materials are alloys of two or more materials which give improved physical and mechanical properties. Practically, in such alloys grain boundary motion without obstacles is the exception rather than the rule. In most of the cases the obstacles are in the form of second phase particles [78-80] or voids present on the grain boundaries [81-83]. However, the effect of second phase particles on grain growth is considerably small for grains which have larger average grain area (in micro scale) in comparison to sub-micron or nano grain size materials. Hence, it seems that the presence of particles in nanosize grained material is likely to have a more profound influence on the microstructural
evolution such as nucleation rate, texture evolution etc. However, this effect depends on the volume fraction of particles or voids present, distribution of particles and the kinetic nature of particles.

Over the past several decades, many theoretical, experimental and computational studies were made on the effect of immobile particles on grain growth [84, 85]. A more complex situation arises when the mobile second phase particles are considered. Nevertheless, this consideration is important as there are examples where particles are pushed by moving grain boundary [42, 43, 45].

We develop and present a phase field model for microstructural evolution in presence of mobile and immobile particles. In section 2, we present an overview of the phase field theory and the discretization technique employed. A short description for the mechanism of grain growth in presence of second phase particles has been discussed in section 3. The driving force for the motion of the particles is considered to be proportional to the curvature of grain boundary. In section 4, we implement the phase field theory for grain growth in presence of mobile particles. In the evolution equation, we introduce a separate order parameter for each particle. The local curvature of the grain boundary is written explicitly in terms of the order parameters. The interpenetration between two neighboring particles is avoided by considering a repulsive force. We briefly describe the computational aspects used in context of simulations with mobile particles in section 5. In section 6, the interaction of a radially symmetric grain boundary with radially symmetrically distributed particles is examined. In section 7, we study the interaction of a single particle in one quadrant of a circular bicrystal. We examine the conditions under which the particle pins the grain boundary or is dragged by the
boundary. Finally, we discussed a bicrystal grain growth in presence of dense second phase mobile particles in section 8.

4.2 Overview of phase field theory

The class of diffuse interface models, the so-called “Phase-field model”, was first originated for the modeling of solidification of a pure melt by Fix [86], Collins and Levine [87] and Langer [88]. The basic concept of that model was replacing of sharp solid-liquid interface by a diffuse interface which is continuously evolved between two equilibrium states (solid and liquid). The advantage of this model is that no boundary conditions are required at the interface; only periodic boundary conditions are applied at the boundary of the domain. The interface movement is described by the temporal evolution of the zero or certain level-set of the phase field.

In this section we briefly describe the theory of multiphase field model developed by Chen and co-workers which is more relevant in a polycrystalline setting. More detailed descriptions of the phase field method may be found in [29-31].

4.2.1. Theory

The phase field theory is a simple phenomenological means of describing evolution of microstructure and employs three essential features: (1) continuous field variables to describe the phase of the material, (2) energy of the system expressed in terms of these field variables, and, (3) an evolution equation (usually a gradient flow type equation) driving the system to minimum free energy.
In the context of polycrystalline materials, the “phases” of the material are the individual grains of unique orientations. Grain growth occurs by means of grain boundary propagation. The model as originally proposed employs as many field variables as there are unique orientations of the grains [30]. A system with $Q$ unique orientations would require $Q$ phase field variables to describe it: $\eta_1(x, t)$, $\eta_2(x, t)$, ..., $\eta_Q(x, t)$, which are functions of material points $x$ and time $t$. The subscripts map each order parameter to a unique orientation of the grains: $\eta_i \to \theta_i$, $i = 1, \ldots, Q$. A presence of a grain of orientation at $\theta_i$ at a point is described by the order parameter $\eta_i$ taking a value 1.0 at that point and all other order parameters taking 0 values. In the absence of diffusion, the order parameters are nonconserved quantities. Note that only discrete grain orientations can be described using a finite number of order parameters. Choosing large number of $Q$ can approximate a continuous distribution of grain orientations.

The total free energy of the system $F$ consists of the coarse-grained free energy $f(\eta_1, \eta_2, \ldots, \eta_Q)$ and a gradient energy $g(\nabla \eta_1, \nabla \eta_2, \ldots, \nabla \eta_Q)$. Thus, the system free energy in the absence of diffusion is written in terms of the order parameters as

$$ F = \int_V \left[ f(\eta_1, \eta_2, \ldots, \eta_n) + g(\nabla \eta_1, \nabla \eta_2, \ldots, \nabla \eta_Q) \right] dV. \quad (4.1) $$

The coarse grained free energy is the bulk energy of the individual grains away from the interfaces. Since the grains differ from each other solely by rigid rotations, the bulk energy per unit volume of all the grains is identical. The coarse grain energy $f(\eta_1, \eta_2, \ldots, \eta_Q)$ is thus chosen to have the form of multi-well potential with each minima of equal depth at different grain orientation. In our simulation, we use the multi-well free energy density functional of Fan and Chen [30].
where the phenomenological parameters are chosen $\alpha = \beta$ and $\nu > \alpha/2$ to allow $2Q$ equal minima to exist. The exact form of free energy density functional $f(\eta_i)$ is not important as long as it gives $2Q$ minima with equal potential well depth at $(\eta_1, \eta_2, \ldots, \eta_Q) = (\pm 1, 0, \ldots, 0), (0, \pm 1, \ldots, 0), \ldots, (0, \ldots, 0, \pm 1)$. The gradient term penalizes sharp interfaces and the competition between the coarse grain energy and the gradient term causes the formation of diffuse interfaces between the grains. The gradient energy is given by

$$\sum_{i=1}^{Q} k_i \left( \frac{1}{2} |\nabla \eta_i|^2 \right) \quad (4.3)$$

where $k_i$ is the gradient energy coefficient.

Substituting equation (4.3) and (4.2) into equation (4.1), the total free energy of the system can be described by the following expression

$$F = \int_V \left\{ \sum_{i=1}^{Q} \left( \frac{\alpha}{2} \eta_i^2 + \frac{\beta}{4} \eta_i^4 \right) + 2\nu \sum_{i=1}^{Q} \sum_{j>i}^{Q} \eta_i^2 \eta_j^2 \right\} + \sum_{i=1}^{Q} \frac{k_i}{2} |\nabla \eta_i|^2 \right\} dV \quad (4.4)$$

The next ingredient of the phase field theory is the evolution equation for the order parameters. In the Ginzburg-Landau framework, this is usually chosen as a simple gradient flow type equation which drives the system to the minimum free energy

$$\frac{\partial \eta_i}{\partial t} = -L_i \frac{\delta F}{\delta \eta_i}, \quad \text{with } i = 1, 2, \ldots, Q, \quad (4.5)$$

where $\delta$ is the variational derivative.

Substituting equation (4.4) in the evolution equations (4.5), we obtain the governing equations for grain growth.
\[
\frac{\partial \eta_i}{\partial t} = L_i \left( k_i \nabla^2 \eta_i + \alpha \eta_i - \beta \eta_i^3 - 4 \nu \eta_i \sum_{j \geq i}^Q \eta_j^2 \right), \quad i = 1, 2, ..., Q. \quad (4.6)
\]

Equation (4.6) is a set of \( Q \) coupled, nonlinear, hyperbolic equations which are solved using the \textit{finite difference} method. For isotropic grain growth, the coefficients \( L_i \) and \( k_i \) are assumed to be constant.

4.2.2 Discretization technique

In order to solve the diffuse interface model numerically, we discretized the Ginzburg-Landau equations (4.6) in space and time at each grid points. The gradient term is discretized using the central difference method.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{discretizationStencil.png}
\caption{Discretization stencil of \( \eta \) at any arbitrary point.}
\end{figure}
Figure 4.1 shows the schematic view of standard nine-point discretization. The Taylor expansion of the first neighbour point of $\eta_{ij}$ yield,

$$
\eta(i \pm 1, j) = \eta(i, j) \pm (\Delta x)\eta_x(i, j) + \frac{(\Delta x)^2}{2!}\eta_{xx}(i, j) + \text{higher term}
$$

(4.7)

$$
\eta(i, j \pm 1) = \eta(i, j) \pm (\Delta y)\eta_y(i, j) + \frac{(\Delta y)^2}{2!}\eta_{yy}(i, j) + \text{higher term}
$$

where subscripts represent partial derivative.

Assume a uniform spacing ($\Delta x = \Delta y \approx \Delta$) for the entire simulation domain. Summing up equations (4.7) yield,

$$
\nabla^2 \eta(i, j) \times \Delta^2 = 4\eta(i, j) + \eta(i + 1, j) + \eta(i - 1, j) + \eta(i, j + 1) + \eta(i, j - 1)
$$

(4.8)

The second neighbours can be expanded by Taylor series as,

$$
\eta(i \pm 1, j \pm 1) = \eta(i, j) \pm (\Delta x)\eta_x(i, j) + (\Delta y)\eta_y(i, j) + \frac{1}{2!}
\left[(\Delta x)^2\eta_{xx}(i, j) \pm (\Delta y)^2\eta_{yy}(i, j)\right] + \text{higher term}
$$

(4.9)

$$
\eta(i \mp 1, j \mp 1) = \eta(i, j) \mp (\Delta x)\eta_x(i, j) - (\Delta y)\eta_y(i, j) + \frac{1}{2!}
\left[(\Delta x)^2\eta_{xx}(i, j) \mp (\Delta y)^2\eta_{yy}(i, j)\right] + \text{higher term}
$$

Equations (4.9) can be written as,

$$
2\nabla^2 \eta(i, j) \times \Delta^2 = \eta(i + 1, j + 1) + \eta(i + 1, j - 1) + \eta(i - 1, j + 1) + \eta(i - 1, j - 1) + 4\eta(i, j)
$$

(4.10)

For simplicity, any arbitrary grid point $(i,j)$ we denote by subscript $i$, and the corresponding first and second nearest neighbours represented by subscript $j$ and $k$ respectively. Thus, the gradient penalty term can be represented from equations (4.8) and (4.10) in the following form:

$$
\nabla^2 \eta_i = \frac{1}{\Delta^2}
\left[\frac{1}{2}\sum_j (\eta_j - \eta_i) + \frac{1}{4}\sum_k (\eta_k - \eta_i)\right], \quad i = 1, 2, ..., Q
$$

(4.11)
The time derivatives are discretized using a forward-Euler difference to obtain an explicit finite difference scheme:

\[ \frac{\partial \eta_i}{\partial t} = \frac{\eta_i(x, t+\Delta t) - \eta_i(x, t)}{\Delta t}, \quad i = 1, 2, \ldots, Q \]  

(4.12)

4.3 Grain growth mechanism in presence of second phase particles

Grain growth is the process by which smaller grains gradually shrink and larger ones grow. This process is the result of a reduction in grain boundary energy and the growth rate is limited by the movement of atoms across the boundary (which governs the grain boundary mobility).

The presence of second phase particles restricts the grain boundary motion and thus controls the grain growth. This situation arises due to the pinning forces exerted by the particle-matrix interface on grain boundary. If \( P_{gg} \) represents the driving force for particle free grain growth and \( P_Z \) represent the total pinning force per unit area of the grain boundary due to the presence static particles, then the grain boundary motion can be expressed as

\[ \frac{dR}{dt} = m_b(P_{gg} - P_Z) \]  

(4.13)

where \( m_b \) is the grain boundary mobility. The motion of the grain boundary will cease if \( P_{gg} = P_Z \). Figure 4.2 shows the interaction between grain boundary and a spherical particle of radius \( r_p \) having incoherent interface. The boundary meets the particle at an angle \( \theta \). The force components arising from the particle and the grain boundary are also shown. Resolving forces in the forward direction, the pinning force by each particle can be expressed as
\[ P_{\text{drag}} = \pi r_p \gamma_b \sin 2\theta \]  

(4.14)

where \( \gamma_b \) is the interfacial energy of the grain boundary. Thus the pinning force depends on the size of the particle and the interaction position between particle and the grain boundary. For a particular size of particle, the maximum pinning force is obtained when grain boundary meets with particle at 45\(^\circ\). It is to be noted that the region of the boundary where the particle interact is lost. Due to the lower energy at the intersection, particles are attracted to boundaries.

\[ b v_m \gamma \kappa = \]  

(4.15)

Figure 4.2: A graphical representation of a bicrystal system for the mechanism of GB migration effected by the pinning of particle. \( \theta \) is the boundary bypass angle; \( \gamma_b \) is the boundary surface tension, \( R \) is the radius of boundary curvature.

The driving force \( (P_{gb}) \) for the grain boundary arises from its curvature. The most general form of the grain boundary migration speed for a small segment of the boundary can be written by the following expression [33]:

\[ v = m_b \kappa \gamma \]  

(4.15)
where $\kappa_{\gamma}$ is the local weighted mean curvature of the boundary. If the boundary energy per unit area is $\gamma$ and local mean curvature is $\kappa$ then the local weighted mean curvature can be expressed as,

$$\kappa_{\gamma} = \gamma \kappa$$  \hspace{1cm} (4.16)

In isotropic setting, the value of $m_b$ and $\gamma$ are taken to be constant.

The velocity of the mobile particles is taken to be proportional to the driving force on the particle due to the curvature of the grain boundary:

$$v_p = m_p \gamma \kappa$$  \hspace{1cm} (4.17)

The mobility constants $m_p$ for various mechanisms of particle motion have been collated by Gottstein and Shvindlerman [72]. A typical expression for the mobility of a solid inclusion with bulk diffusion in the matrix as the dominant mechanism of atomic transport is given by Geguzin and Krivoglaz [89]

$$m_p = \frac{D_{\text{vol}} \Omega}{k_B T r_p^3}$$  \hspace{1cm} (4.18)

where $D_{\text{vol}}$ is the diffusion coefficient in the bulk, $\Omega$ is the atomic volume, $k_B$ is the Boltzmann constant, $T$ is the temperature and $r_p$ is the radius of the particle. If interface diffusion is the dominant mechanism, the mobility is proportional to $r_p^{-4}$. Thus the mobility is strongly dependent on the particle radius.

The local curvature $\kappa$ of the grain boundary is evaluated using

$$\kappa = \text{Div}\ n$$  \hspace{1cm} (4.19)

where $n$ is the normal of the grain boundary.
4.4 Phase field model implementation

In this section, we develop the governing equations for the kinetics of grain boundary in presence of mobile particles. Recently, Moelans et al [39, 40] have proposed a modification to the phase field theory for grain growth to account for the presence of immobile particles. They include a single additional phase field variable $\eta(x)$ in the free energy functional to represent all the particles. Thus, the free energy density functional is the sum of free energy functional for the grain matrix and particles,

$$f = f_m + f_p$$  \hspace{1cm} (4.20)

where $f_m$ is the local free energy density inside of the matrix phase of grains and $f_p$ stands for local free energy density inside of the particles and are the functions of order parameters. In contrast to the order parameters describing the grains, the variable describing the particles does not evolve and is independent of time. In our case since the particles are mobile, it is convenient to introduce a separate order parameter field for each particle. This will help to track the individual particles easily and avoid interpenetration of particles. Since $\eta_i$, $i = 1, \ldots, Q$ represent the grains we use the variables $\eta_i$, $i = Q + 1, \ldots, Q + p$ to represent $p$ particles. Thus the free energy for the particles can be expressed as,

$$f_p(\eta_1, \eta_2, \ldots, \eta_Q) = \varepsilon \sum_{i=1}^{Q} \sum_{k=Q+1}^{Q+p} \eta_i^2 \eta_k^2$$  \hspace{1cm} (4.21)

where the coefficient $\varepsilon$ represents the interaction between grains and particles.

The modified free energy functional for the system can be obtained from equation (4.2), (4.20) and (4.21),
\[ f(\eta_1, \eta_2, \ldots, \eta_Q) = \sum_{i=1}^{Q} \left( -\frac{\alpha}{2} \eta_i^2 + \frac{\beta}{4} \eta_i^4 \right) + 2\nu \sum_{i=1}^{Q} \sum_{j > i} \eta_i^2 \eta_j^2 + \varepsilon \sum_{i=1}^{Q} \sum_{k=Q+1}^{Q+p} \eta_i^2 \eta_k^2 \]  \quad (4.22)

The phenomenological term is assumed \( \varepsilon = \nu \). The local free energy density for particle has one minima inside of the particles only at \( \eta = (0, 0, \ldots, 0) \). Figure 4.3 represent the local free energy functional inside and outside of the particle for one phase field variable for \( \alpha = \beta = \nu = \varepsilon = 1 \).

The total free energy of the system \( F(\eta) \) now can be expressed using equations (4.3) and (4.22) into equation (4.1):

\[
F = \int \left[ \sum_{i=1}^{Q} \left( -\frac{\alpha}{2} \eta_i^2 + \frac{\beta}{4} \eta_i^4 \right) + 2\nu \sum_{i=1}^{Q} \sum_{j > i} \eta_i^2 \eta_j^2 + \varepsilon \sum_{i=1}^{Q} \sum_{k=Q+1}^{Q+p} \eta_i^2 \eta_k^2 + \sum_{i=1}^{Q} \frac{k_i}{2} \left| \nabla \eta_i \right|^2 \right] dV
\]  \quad (4.23)

where \( k_i \) is the gradient energy coefficient. The evolution for microstructures is obtained by minimizing of total free energy of the system. Employing the time-dependent
Ginzburg-Landau equation for nonconserved order parameter [18] the following form of evolution equations are obtained,

\[
\frac{\partial \eta_i}{\partial t} = L_i \left( k_i \nabla^2 \eta_i + \alpha \eta_i - \beta \eta_i^3 - 2 \eta_i \left( 2 \nu \sum_{j=1}^{Q} \eta_{j}^2 + \varepsilon \sum_{k=Q+1}^{Q+p} \eta_{k}^2 \right) \right) \quad \text{with } i = 1, 2, \ldots, Q. (4.24)
\]

where \( L_i \) is the kinetic coefficient parameter which represent the mobility of grain boundaries. For isotropic evolution, the gradient energy coefficient \( k_i = k \) and kinetic coefficient \( L_i = L \) for all \( i \).

In order to describe the motion of the particles we consider a constitutive kinetic relation for each particle of the form given by Eq. (4.19). The local curvature of the grain boundary of the \( i \)-th grain is given by

\[
\kappa = \text{Div} \mathbf{n} = \text{Div} \left( \frac{\nabla \eta_i}{|\nabla \eta_i|} \right)_{\mathbf{x} \in \partial \mathbb{R}} \quad (4.25)
\]

where \( \mathbf{n} \) is the normal to the grain boundary \( \partial \mathbb{R} \) at the boundary of the particles. The curvature of the \( i \)-th grain may be written explicitly in terms of the order parameters as

\[
\kappa = \left\{ \frac{\eta_{i_{xy}} \eta_{i_x}^2 - 2 \eta_{i_x} \eta_{i_x} \eta_{i_{xy}} + \eta_{i_{xx}} \eta_{i_x}^2}{\left( \eta_{i_x}^2 + \eta_{i_y}^2 \right)^{3/2}} \right\} \quad (4.26)
\]

where the subscripts \( x \) and \( y \) represent derivatives.

Thus using Eq. (4.17), (4.18) and (4.26), the constitutive relation for the velocity of the \( k \)-th particle can be written explicitly as

\[
\frac{d \mathbf{r}_k}{dt} = \frac{M}{r_p^3} \left\{ \frac{\eta_{i_{yy}} \eta_{i_x}^2 - 2 \eta_{i_x} \eta_{i_y} \eta_{i_{xy}} + \eta_{i_{xx}} \eta_{i_x}^2}{\left( \eta_{i_x}^2 + \eta_{i_y}^2 \right)^{3/2}} \right\} \quad (4.27)
\]
where $r_k$ is the position vector of the center of the $k$-th particle and $M = D_{vol} \Omega \gamma / k_b T$ is a constitutive coefficient which depends on the mechanism of particle motion.

To avoid the interpenetration of the particles we also employ an inter-particle repulsive force between particles $i$ and $j$ of the form,

$$ f_{ij} = \frac{C}{|r_i - r_j|} n_{ij}, \quad i \neq j \tag{4.28} $$

where $C$ is a constant and $n_{ij} = (r_i - r_j)/\|r_i - r_j\|$ is a unit vector in the direction of the line joining the centers of the particles. This force is insignificant when the particles are apart but repels overlapping particles. The above expression mimics the classical hard sphere potential but is computationally simpler to implement.

4.5 Computational aspects

To study grain growth, the Ginzburg-Landau equations (4.24) are solved numerically by discretizing in space and time. Periodic boundary conditions were employed. Area and radius of the grain are calculated by the number of grid points (g.p) and time in number of time steps. Equation (4.27) is discretized to move the particle according to the constitutive equation (4.17). Though $\kappa$ represents the curvature of the grain on the boundary of the particle, for computational purposes we calculate the average value of $\kappa$ in small neighborhood of the particle. We check the accuracy of the curvature thus obtained by comparing with a single particle interacting with a circular grain boundary.

Following Fan and Chen [30] we take the values $\alpha = 1$, $\beta = 1$, $\gamma = 1$, $\kappa = 2$, $L = 1$, $\varepsilon = 1$, $\Delta t = 0.25$, $\Delta x = \Delta y = 2.0$. Periodic boundary conditions are applied in both $-x$ and $-y$
directions of the simulation domain. To visualize the microstructure evolution of bicrystal with time using phase-field variable, we define the following function:

\[ \varphi(x, t) = \sum_{i=1}^{O} \eta_{i}^{2}(x, t), \quad \eta_{i} = 1, 2, \ldots, O \]  

(4.29)

which takes values of unity inside of the grain matrix and a significantly smaller positive values across the grain boundaries.

4. 6 Interaction of grain boundary with axisymmetric distribution of particles

First, we consider a circular grain embedded in an infinite grain and a radially symmetric dense distribution of particles as shown in figure 4.4.

The circular grain shrinks in order to reduce the grain boundary energy and the total free energy of the system. In the absence of the particles, the grain shrinks according to the classical law

\[ R(t)^{2} - R_{o}^{2} = 2m_{b} \gamma_{b} t , \]  

(4.30)

Figure 4.4: Circular grain containing embedded by an infinite grain. Particles are distributed radially inside of the circular grain.
where \( R(t) \) is the current radius of the grain at time \( t \) and \( R_0 \) is the initial radius. We treat the dense uniform distribution of particles as a single radially symmetric annular ring particle. In this case, \( \eta(x, t) = \eta(r, t), i = 1, 2, 3 \) and the governing equations (4.24) reduce to the axisymmetric form

\[
\frac{\partial \eta_1}{\partial t} = L \left\{ \kappa \left( \frac{\partial^2 \eta_1}{\partial r^2} + \frac{1}{r} \frac{\partial \eta_1}{\partial r} \right) + \alpha \eta_1 - \beta \eta_1^3 - 2 \nu \eta_1 \eta_2^2 - 2 \epsilon \eta_1 \eta_3^2 \right\},
\]

\[
\frac{\partial \eta_2}{\partial t} = L \left\{ \kappa \left( \frac{\partial^2 \eta_2}{\partial r^2} + \frac{1}{r} \frac{\partial \eta_2}{\partial r} \right) + \alpha \eta_2 - \beta \eta_2^3 - 2 \nu \eta_1 \eta_2^2 - 2 \epsilon \eta_2 \eta_3^2 \right\}, \tag{4.31}
\]

where \( \eta_3 \) represents the annular particle. We thus specify

\[
\eta_3(r, 0) = \begin{cases} 
1, & r_0 - \frac{r_p}{2} < r < r_0 + \frac{r_p}{2} \\
0, & r_0 + \frac{r_p}{2} < r < r_0 - \frac{r_p}{2} 
\end{cases} \tag{4.32}
\]

where \( r_0 \) is the initial location of the center of the particle and \( r_p \) is the width of the annular ring particle. For the axisymmetric grain boundary, the driving force is simply \( \gamma_b / R(t) \) in the absence of particles. When the grain boundary interacts with the particles the driving force changes to \( \gamma_b' / R(t) \) where \( \gamma_b' \) is the grain boundary energy in the presence of the particles. Thus even in the presence of particles the grain boundary evolution is similar to Eq. (4.30) but with different mobility coefficient and grain boundary energy.
In figure 4.5, we plot the field $\phi(r) = \eta_1^2 + \eta_2^2$ as a function of radial position at different times. Inside each grain $\phi = 1$ and on the grain boundaries $\phi < 1$. Figure 4.5(a) shows the shrinking grain boundary locations in the absence of particles. The grain boundary accelerates due to the increase in driving force at smaller radii of curvatures. Figure 4.5(b) shows the grain boundary pinned by an immobile particle of radius $r_p = 3$ located at $r_0 = 140$ whereas figure 4.5(c) shows the grain boundary dragging along a mobile particle of radius $r_p = 3$ initially located at $r_0 = 140$ (all length scales are in grid units). In this case, the grain boundary velocity is governed by the mobility of the particle. Note that the grain boundary detaches from the mobile particle at small radius. This is due to the fact that increase in energy of the system due to particle detachment is compensated.
by the decrease in energy due to faster (particle free) grain boundary motion. The grain boundary detaches from the particle at a radius \( R = 14 \) for the assumed value of the particle mobility. For an immobile particle, the detachment of the grain boundary occurs when the particle is located at \( R = 17 \). This is also predicted by the theoretical energy bifurcation analysis presented in Chapter 3 in the context of particles distributed uniformly throughout both grains. We adapt this analysis for our annular ring distribution of particles.

The grain boundary has two choices at every instant of time. It can drag the particles along with it or snap through leaving them behind. Each of these choices allow the grain boundary to move by different velocities. We assume that the choice leading to smaller total energy for the system at time \( t + \Delta t \) is chosen by the grain boundary. In the event that the particles are shed by the grain boundary, the change in energy of the system is given by

\[
\Delta E_1 = 2\pi R_1(t + \Delta t) L \gamma_b - 2\pi R(t) L \gamma'_b
\]  

(4.33)

where \( R_1(t + \Delta t) \) is the radius of the grain boundary at time \( t + \Delta t \) assuming that it moved with the particle free velocity \( v_b = -m_b \gamma_b / R \). We have set \( \gamma_b \) and \( \gamma'_b \) to be the grain boundary energy per unit surface area in the absence and presence of particles, respectively. On the other hand, if the grain boundary drags the particles along, the energy is given by

\[
\Delta E_2 = 2\pi v_p L \gamma'_b \Delta t
\]  

(4.34)

where \( v_p = -m_p \gamma'_b / R \) is the loaded grain boundary velocity.
The choice of whether the boundary sheds the particles or drags them along depends on whether $\Delta E_1$ or $\Delta E_2$ is larger. Particles are shed if $\Delta E_1 < \Delta E_2$ and are dragged along if $\Delta E_1 > \Delta E_2$. This choice arises because the increase in the total energy due to shedding of the particles is compensated by the decrease in grain boundary energy due to faster particle-free grain boundary motion. Since the grain boundary has to move a minimum distance of the size of the particle (width of the annular ring) in order to shed the particles we obtain

$$\Delta t = \left| \frac{\lambda r_p}{v_b} - \frac{\lambda r_p R}{m_b \gamma_b} \right|$$

where $\lambda \in (0, 2)$ is a geometric parameter which depends on where the particle intersects the grain boundary. Substituting $R_l(t + \Delta t) = R(t) - m_b \gamma_b \Delta t / R(t)$ in Eq. (4.33), we solve the Eqs. (4.33) and (4.34) to obtain the critical radius at which the grain boundary snaps through the annular ring particle as

$$R^* = \frac{\lambda r_p}{1 - \gamma_r} \left(1 - m_r \gamma_r^2\right)$$

where we have set $m_r = m_p / m_b$ and $\gamma_r = \gamma'_b / \gamma_b$ for convenience. Thus the critical radius at which the grain boundary snaps through the particle decreases linearly with the particle mobility. We test this prediction numerically using the phase field model and find that the detachment radius decreases linearly with particle mobility (figure 4.6).

Figure 4.7 shows the grain boundary position with time for the three cases: particle free evolution, immobile particle and mobile particle with $M = 20$. In the absence of the particles, the grain boundary evolves according to Eq. (4.30). In the presence of both the immobile and mobile particles, the grain boundary first evolves in a particle free manner away from the particle. As the grain boundary approaches the particle, it is momentarily attracted by the particle as marked by the arrow in figure 4.7. Thereafter, the grain
boundary is either pinned (in the immobile particle case) or moves at a reduced velocity (in the mobile particle case). The detachment of the mobile particle from the grain boundary at small radius can also be seen in the figure. The velocity of the grain boundary is plotted with position in figure 4.8. The attraction of the grain boundary to the particle in the immobile and mobile cases is apparent in the figure. The detachment of the grain boundary from the mobile particle and the subsequent acceleration to the particle free velocity at latter stages is also clearly seen in this figure.

Figure 4.6: Critical radius at which the grain boundary detaches from the particle vs particle mobility.
Figure 4.7: Radius of the inner circular grain with time. The dash-dotted line is the particle free grain evolution. The dashed line is the grain boundary pinned by the immobile particle. The solid line shows the slowing of the grain boundary due to the presence of the mobile particle. The arrow indicates the initial attraction of the grain boundary to the particle.

Figure 4.8: Velocity of the grain boundary vs position. The solid line is the loaded grain boundary and has lower velocity than the particle free grain boundary (dash-dotted line). The initial peak is due to the attraction of the grain boundary as it approaches the particle.
4.7 Interaction of grain boundary with single mobile and immobile particle

In this section we examine the interaction between a bicrystal grain boundary and a single particle in a two-dimensional setting. For the sake of simplicity and computational convenience, we consider one quadrant of a circular grain embedded in another grain. Initially the particle is located inside the circular grain at radial distance \( d \) from the center as shown in figure 4.9. Since the grain boundary is driven by a force proportional to its curvature towards its center of curvature, the circular grain is expected to shrink. When the grain boundary is far from the particle, it experiences particle free motion. On the other hand, when the grain boundary intersects with the particle, it is either pinned by the particle or drags it along or detaches from the particle.

![Figure 4.9: Sketch of bicrystal in presence of particles. (a) Circular grain embedded by another grain in presence of four particles (b) Quarter portion of the circular grain with one particle.](image)

The temporal evolution of the bicrystal system in presence of second phase immobile particle is shown in figure 4.10(a). The particle size is \( r_p = 2.5 \) (grid units) and the initial distance of particle is \( d = 170 \) (grid units) from the center of the circular grain while the initial radius of the circular grain is \( R = 180 \). When the grain boundary approaches the particle, it is locally attracted to it as seen by the formation of a dimple at \( N = 1000 \). The
particle pins the grain boundary up to $N = 12000$ time steps. The boundary away from the particle continues to evolve, increasing the curvature near the particle. The grain boundary then detaches from the immobile particle when its curvature (and hence its driving force) becomes large near the particle and exceeds the particle pinning force. In figure 4.10(b), the evolution of the grain boundary in the presence of a mobile particle is shown. The mobility coefficient is chosen to be $M = 50$ with particle radius $r_p = 2.5$. It can be observed that the grain boundary drags the mobile particle and since the mobility of the particle is high enough, the grain boundary maintains its initial circular shape. In figures 4.10(c) and 4.10(d), we present the evolution of bicrystal in presence of second phase immobile and mobile particles respectively in the presence of a larger particle ($r_p = 3.0$). Compared to the evolution in figure 4.10(a) and 4.10(b), it can be observed that the evolution is affected by the size of the particle. When the particle size is increased, the kinetics of grain boundary becomes much slower. In fact, for immobile particle the grain boundary is stuck and does not become free even after long time. In figure 4.10(d), the effective mobility of the particle is smaller than in figure 4.10(b) (due to larger particle size) and hence the curvature near the particle is larger so that the particle velocity matches the grain boundary velocity away from the particle.
Figure 4.10: Comparison for the motion of the grain boundary in presence of (a) an immobile particle and (b) mobile particle with mobility coefficient $M = 50$. The particle size is $r_p = 2.5$ in both cases. In (c) and (d), the interaction of the gain boundary with immobile and mobile particles of size $r_p = 3.0$ respectively is shown.
In figure 4.11(a), we plot the temporal evolution of the average radius $R_{\text{ave}} = \sqrt{4A/\pi}$ of the inner grain, where $A$ is the area of the inner grain in grid points. The particle free case is shown using the solid line, immobile particle case is shown using the dash-dotted line and the mobile particle case is shown using the dashed line. The particle size is $r_p = 2.5$ in both cases. The attraction of the grain boundary and the particle is seen from the fact that the average radius is smaller for the simulations with the particles than the particle free case (more clearly seen in figure 4.11(b)). The pinned regime and the detachment (marked with an arrow) of the grain boundary for the immobile case can also be seen in figure 4.11(a).

![Figure 4.11](image)

Figure 4.11: (a) The plot of average radius of the inner grain vs simulation time for particle free GB motion (solid line) and GB motion in presence of mobile (dashed line) and immobile particle (dash-dot line) of particle radius $r_p = 2.5$. The arrow indicates the detachment of the grain boundary from the particle. Figure (b) is a closer view of the dotted rectangle in (a) showing the acceleration of the grain boundary due to attraction to the particle.

The evolution of the grain in the presence of mobile particle with very low mobility $M = 2.5$ is shown in figure 4.12. The low mobility of the particle causes the local curvature of
the grain boundary near the particle to increases. When the curvature increases beyond the pinning force of the particle, the grain boundary detaches.

In figure 4.13(a), the effect of particle size on the grain evolution is shown. As expected, for larger particles, the effective particle mobility is smaller and this causes the inner grain to shrink more slowly. Similarly, when the mobility coefficient $M$ is decreased, the effective rate of evolution of the inner grain is smaller (figure 4.13(b)). At low mobility coefficient, the grain detaches from the particle as shown by the arrow in figure 4.13(b).
Figure 4.13: Average radius of the inner grain as function of simulation time in the presence of single mobile particle: (a) effect of variation of particle size (b) effect of mobility coefficient ($M$).
4.8 Bicrystal interaction with dense mobile particles

In this section, we present some results of a bicrystal model in presence of dense mobile particles. Figure 4.14 represents the effect of randomly distributed dense mobile particles (6% vf) on bicrystal evolution of size 256×256. The radius of particles are taken as $r_p = 1.5$ while the mobility of particles was taken $M = 100$. It was clearly observed that the particles are swept from the grain matrix and accumulated on the grain boundary. The density of the particles on the grain boundary increases with the increase of simulation time. A clear particle free band behind of the grain boundary was observed. This dragging of particles by grain boundary is quite natural if the particles are mobile and is comparable with the experimental evidence of the Ashby and Gentamore [42].

![Figure 4.14: 2-D evolution of grain shrinkage in presence of 6% vf mobile impurities with $M=100$: (a) initial microstructure (b) $N = 400$ (c) $N = 800$ (d) $N = 1200$.](image)

Figure 4.14 exhibits the effect of particles mobility on the reduction of average radius for the circular grain. Results are simulated by considering a quarter of the circular grain. The particles’ hindrance on the growth process is more pronounced with decrease of the mobilities of the particles.
4.9 Conclusions

A unified simple numerical model for bicrystalline grain growth in presence of mobile and immobile particles is presented. A constitutive kinetic relation is assumed for the mobile particle by which the velocity of the particle is assumed to be proportional to the driving force due to the curvature of the grain boundary. The proportionality constant is the mobility coefficient which is inversely proportional to the third or fourth power of the particle radius depending on the mechanism of atomic transport by which the particle mobility occurs. The computational implementation of the phase field model is described.
and simulations are shown in a one-dimensional axisymmetric setting as well as in two-dimensional bicrystal evolution via grain boundary migration.

It is observed that the presence of particle adversely affects the process of evolution of the grain. The grain boundary motion increases near the particle due the attraction force of the particle. As the mobility of the particle is inversely proportional with the particle radius, the kinetics of grain boundary is much affected with increase of the particle size. For larger immobile particle size ($r_p = 3.0$) the grain boundary is totally stuck and the evolution of the grain is stopped. Depending on the size and the mobility of the particle, the grain boundary can leave behind the particles. In the case of dense mobile particles, the particle free band behind the grain boundary corresponds very well with the experimental observation of Ashby and Gentamore [42, 43] for particle dragging by the grain boundary.
CHAPTER – 5

Phase field simulation for grain growth in polycrystalline materials

5.1 Introduction

This chapter presents a computational model to investigate the grain growth for polycrystalline materials. In phase field simulations of polycrystalline grain growth a large number of order parameters are required to describe the individual grains. The concomitant computational expense has restricted previous studies to small numbers of order parameters and, implicitly, the misorientation angles between adjacent grains to a small finite number of discrete values. The treatment of large number of order parameters and continuous misorientation angles is made possible here using the active parameter tracking (APT) algorithm proposed by Vedantam and Patnaik [38]. We investigate the polycrystalline grain growth with isotropic and anisotropic grain boundary energy using APT algorithm.

Most of the metals and metallic alloys are highly anisotropic where grains are randomly oriented relative to each other. Hence, it would be appropriate to first learn more about how anisotropy influences the growth kinetics and thus the mechanical and physical behavior of materials. However, so far, most of the literature study (theoretical, experimental, and computational) mainly focused to understanding the grain growth behavior in the isotropic limit where the grain boundary energy and mobility are considered to be constant [30, 90-93].
The grain boundary anisotropy means that the energy and mobility of the grain boundaries are strongly dependent on the grain boundary misorientation and inclination. It is well known that the adjacent grains have different lattice orientations with respect to a fixed axis and the interfaces between the grains are the grain boundaries. The coordination number (number of neighbors) of atoms on the grain boundaries is different from that of the bulk atoms and this modifies the energy per atom on the boundaries. In addition, preponderance of grains of certain orientations provides a texture to the material and this has a significant effect on the bulk material properties as well. Inside each grain, the atoms are arranged in a crystalline lattice in the absence of vacancies or dislocations. However, on the grain boundaries, the crystalline order is lost and the mismatch between the different lattice orientations of the adjacent grains is accommodated through the presence of dislocations. This results in an increase of energy per atom on grain boundaries relative to atoms inside the grains. The number and distribution of the dislocations, and hence the energy of the atoms on the boundaries, is dependent on the misorientation of the adjacent grains [94]. In two dimensions the angle between the lattice axes of adjacent grains represents the misorientation of the grains. Under certain conditions such as sufficiently high temperatures, the grain boundaries propagate and the larger grains grow at the expense of smaller grains to minimize the total grain boundary energy of the material [95]. If the grain boundary energy is assumed to be independent of the misorientation (isotropic grain boundary energy), the growth rates of the average grain radius $<R_{ave}>$ is given by the power law $<R_{ave}> \sim t^{1/2}$. In anisotropic situations, the growth rates are significantly different. Since microstructural features such as the grain
size and orientation determine the mechanical properties of the material, an understanding of these features is essential for obtaining desired mechanical properties.

The phase field method has added advantages in introducing size, time, temperature more directly in comparison to other computational methods. However, so far, most phase field studies have focused on isotropic systems or anisotropic systems restricted to low misorientations [8, 35, 96]. This is mainly due to the fact that the most popular variant of the phase field approach — the multiphase field method — requires a different order parameter for each grain of different orientation. The computational expense of using many order parameters has hitherto precluded a wide range of grain orientations. Moreover, using small number of order parameters permits artificial coalescence when grains of the same orientation come into contact during grain growth. The computational restriction on the number of order parameters allowed is overcome by using an algorithm proposed recently by Vedantam and Patnaik [38] (and independently by Gruber et al [97] and Kim et al [98]). An alternative, computationally complex, approach is that of dynamic grain reassignment [31, 36].

The central objectives of this chapter are to solve the phase field model for polycrystalline grain growth using a new approach (active parameter tracking algorithm). We study the effect of anisotropy of grain boundary energy on microstructure evolution rates. We find that energy anisotropy delays the growth rate and broadens the scaled grain size with the edge number distribution. Furthermore, in contrast of the previous studies [32, 35], our energy anisotropy is not restricted to low misorientation angles between adjacent grains. We find that the decrease in the growth rate for anisotropic grain boundary energy is more pronounced in the presence of high angle grain boundaries.
which are described using an extension of the Read-Shockley form for the grain boundary energy\[50\].

5.2 Grain boundary energy anisotropy

For isotropic grain growth, the coefficients $L_i$ and $k_i$ are assumed to be constant. To incorporate misorientation dependence of grain boundary energy, the gradient coefficient $k$ is related to the grain boundary energy $E_{gb}(\Delta \theta_j)$ (where $\Delta \theta_j = \theta_i - \theta_j$ is the misorientation between grains $i$ and $j$) by choosing $k_i = k_j \propto E_{gb}(\Delta \theta_j)^2$ [96]. This modification entails two changes over the isotropic case: (1) $k_i$ is now an implicit function of position and (2) the grain boundary thickness $\tau$ which is related to $k$ and the barrier height between the wells $\Delta f$ through $\tau \propto \sqrt{k/\Delta f}$ is affected (see Fig 4.3). The latter change is accounted for by scaling $\Delta f$ such that $k/\Delta f = \text{constant}$ to maintain a fixed interface thickness. Since $k_i$ is a function of position, Eq. 4.5 becomes

$$\frac{\partial \eta_i}{\partial t} = L_i \left( \text{div}(k_i \text{grad} \eta_i) + \alpha \eta_i - \beta \eta_i^3 - 4\nu \eta_i \sum_{j>1}^{Q} \eta_j^2 \right), \quad i = 1,2,\ldots,Q. \quad (5.1)$$

5.3 Active parameter tracking algorithm

In the classical algorithm, all $Q$ equations corresponding to all the grains in the domain are solved at every grid point. An alternative method proposed in [38] called the active parameter tracking (APT) algorithm allows the use of unlimited number of order parameters at no additional computational cost. We employ the APT algorithm in our simulations. We briefly describe the APT algorithm below in the context of simulations in the presence of second phase particles. Additional details may be found in [38].
The influence of a grain is only present in a highly localized region near the grain boundaries. Based on this observation, a new algorithm which solves only the active parameters has been proposed [38]. Instead of considering all order parameters at every grid point, only the nonzero order parameters (the active parameters) are solved. Note that the number of active parameters at each grid point may be different. Adjacent grid points may have different sets of order parameters depending on the influence of the local grains. At each point \( x \) and time \( t \), the active phase field variables \( \xi_i, \quad i = 1, 2, ..., Q_a(x,t) \) and the corresponding diffuse order parameter values \( \eta_i, \quad i = 1, 2, ..., Q_a(x,t) \) are stored in memory.

The evolution equations (4.6) can now be written as,

\[
\frac{\partial \eta_{\xi_i}}{\partial t} = L_{\xi_i} \left( \text{div} \left( k_{\xi_i} \text{grad} \eta_{\xi_i} \right) + \alpha \eta_{\xi_i} - \beta \eta_{\xi_i} \eta_{\xi_i} - 4v \eta_{\xi_i} \sum_{\xi_j > \xi_i} \eta_{\xi_j}^2 \right),
\]

where, \( \xi_i = 1, 2, ..., Q_a \) and \( \xi_i \leq Q \).

The number of equations now to be solved at any given point \( Q_a(x, t) \) is much smaller than that for classical algorithm. The number of equations to be solved is usually on the order of 10 or less in initial simulation times and 5 or less at later times. The initial condition is conveniently specified by means of overlapping random shaped regions of different order parameters akin to random initial seeding. This approach allows the use of unlimited number of order parameters and moreover, \( \xi_i \) can be used to represent actual grain orientation angles \( \theta \) to arbitrary precision.
5.4 Simulation procedures

For the evolution of microstructure, the equations (5.2) are solved numerically by discretizing in space and time. The left term of equation (time derivatives) are discretized explicitly using first-forward-Euler difference scheme

\[
\frac{\partial \eta_{\xi_i}}{\partial t} = \frac{\eta_{\xi_i}(x, t + \Delta t) - \eta_{\xi_i}(x, t)}{\Delta t}, \quad i = 1, 2, ..., Q_d \quad \text{and} \quad \xi_i \leq Q.
\]  

(5.3)

The gradient term of the equation (5.2) was discretized by central difference scheme using equal spacing (\(\Delta x\)) in \(-x\) and \(-y\) directions. For complete description of the gradient term, two level discretization was employed

\[
\nabla^2 \eta_{\xi_i} = \frac{1}{(\Delta x)^2} \left[ \frac{1}{2} \sum_{j \neq \xi_i} (\eta_{\xi_j} - \eta_{\xi_i}) + \frac{1}{4} \sum_{k \neq \xi_i} (\eta_{\xi_k} - \eta_{\xi_i}) \right]
\]

(5.4)

Subscript, \(j\) and \(k\) represent first and second nearest neighbors of \(i\)-th grid point. It is to be noted that in explicit schemes, the stability of the simulation process is governed by the time step chosen. Despite this drawback, we prefer this simple scheme to illustrate the proposed strategy of implicit boundary tracking via active parameter tracking algorithm.

For the ease of simulation, the coarse grain energy and mobility coefficient are to be chosen the same values of Fan and Chen [30] as \(\alpha = \beta = L_i = 1.0\). The time step was \(\Delta t = 0.25\) and the spatial steps were chosen to be \(\Delta x = \Delta y = 2.0\). The energy of the grain boundary has been calculated based on dislocation models for low angle grain boundaries [99]. When the misorientation between adjacent grains is small, the distances between dislocations on the grain boundary is large and the grain boundary energy is the sum of the energies of individual dislocations. A widely used expression for the grain boundary energy for \textit{low misorientations} arises from the Read-Shockley model [99].
$\frac{E(\Delta \theta)}{E_0} = \begin{cases} 
\frac{\Delta \theta}{\Delta \theta_m} \left( 1 - \ln \left( \frac{\Delta \theta}{\Delta \theta_m} \right) \right), & \Delta \theta < \Delta \theta_m \\
1, & \Delta \theta \geq \Delta \theta_m 
\end{cases}$ \hspace{1cm} (5.5)

where $E(\Delta \theta)$ is the grain boundary energy and $E_0$ is a constant. $\Delta \theta$ is the misorientation and $\Delta \theta_m$ is the maximum misorientation for which the Read-Shockley formula holds. We take the normalized extended form of Read-Shockley energy formula for large misorientation angles as [50]

$$\frac{E(\Delta \theta)}{E_0} = \sin(2\Delta \theta)(1 - a \ln[\sin(2\Delta \theta)])$$ \hspace{1cm} (5.6)

where $a$ is a constant. Following [100] we take $a = 0.683$. The extended Read Shockley energy is plotted along with the Read-Shockley and isotropic energy in figure 5.1.

Figure 5.1: Energy vs misorientation angle for isotropic (■), Read-Shockley (5.4) (▲) and extended Read-Shockley (5.5) (●) expressions.
5.5 Results and discussion

In this section we examine the effect of energy anisotropy on the evolution of grain growth and the results were compared with isotropic grain boundary energy. We solve the governing equations (5.1) in a $512 \times 512$ square domain using an explicit finite difference scheme. The initial condition is specified by means of approximately 1200 unique randomly sized grains with random orientations. In the isotropic case, the gradient coefficient is assumed to be constant ($k = 2.0$) whereas in the simulations with Read-Shockley (RS) and extended Read-Shockley (ERS) grain boundary energies, the gradient coefficient and the maximum barrier between the wells are scaled by the square of the grain boundary energy.

In order to pictorially represent the grains, it is convenient to define a scalar function of the order parameters,

$$
\varphi(x, t) = \sum_{i=1}^{Q_d} \eta_{\xi_i}^2(x, t), \quad \xi_i = 1, 2, \ldots, Q_d(x, t).
$$

The field $\varphi$ takes values of unity inside each grain and is less than one in the grain boundary region. Contours of $\varphi(x, t)$ are shown in figure 5.2 at three different time steps ($N$): the top row is at $N = 1000$, and the middle row is at $N = 10000$ and the bottom row shows the contours at the $N = 20000$ time step. Columns $(a)$, $(b)$ and $(c)$ in figure 5.2 represent the isotropic grain boundary energy, RS energy and the ERS energy respectively. It can be seen the RS energy (column $(b)$) shows a smaller grain growth rate compared to the isotropic case (column $(a)$). The ERS case shows the smallest grain sizes at the end of the simulation. The grain shapes do not show any significant differences and the number of neighbors per grain appears similar in all three cases. It can be observed
that there are a greater proportion of smaller and larger grains in the anisotropic cases compared to the isotropic case thus showing the effect of anisotropy on the texture evolution. It can also be noted that the interface thickness is independent of the misorientation in the anisotropic cases as expected. The use of unique grain orientations for each grain does not allow coalescence as seen from the lack of abnormal shaped grains.

![Microstructure evolution using isotropic (a), Read–Shockley (b) and extended Read-Shockley (c) GB energy. The top row shows the contours at a time step $N = 1000$ and the middle row is at $N = 10000$ and the bottom row is at $N = 20000$.](image)

Figure 5.2: Microstructure evolution using isotropic (a), Read–Shockley (b) and extended Read-Shockley (c) GB energy. The top row shows the contours at a time step $N = 1000$ and the middle row is at $N = 10000$ and the bottom row is at $N = 20000$. 


Figure 5.3 shows the evolution of the average grain radius with time. The squares represent the isotropic grain evolution and the triangles and circles represent the cases with RS and ERS energies respectively. The growth rate of average radius of the grains is approximated by a simple power law by $\langle R \rangle_t^m - \langle R \rangle_0^m = \alpha t$. The growth exponent $m = 2.02$ for the isotropic case, which is the close to the classical grain growth exponent ($m = 2.0$). The growth exponents of anisotropic grain boundary energies are approximately 2.36 and 2.45 for RS and ERS, respectively. The growth exponents are obtained by fitting the power law using the least squares method for the later stages of grain evolution. Fig. 5.4 shows later time linearity in the log-log plot indicating the power law dependence. Thus the anisotropy of the grain boundary energy delays the growth rate in the RS case [33, 34, 96, 101] and significantly more so in the ERS case.

![Figure 5.3: Average grain radius (grid points) vs Time steps. Square symbols (■) represent the isotropic case and the triangles (▲) and circles (●) represent the RS and ERS cases respectively. The solid lines are the fitted curves.](image)
Figure 5.5 represents the distribution of neighboring grains which is a quantitative indication of the microstructure. The figure shows the distribution at a simulation time steps, \( N = 15000 \) for the isotropic (■), RS (▲), and ERS (●) grain boundary energy. It can be seen that the anisotropic cases are not significantly different from the isotropic case. The similar observation was observed by Kazaryan et.al [96]. Thus the anisotropy of the grain boundary energy does not affect the distribution of the number of neighboring grains.

Figure 5.6 represents the normalized frequency distribution of the normalized grain size after 20000 time steps. As expected, the peak of the frequency for isotropic grain boundary was not shifted. However, the peak of normalized frequency on the size of grains for anisotropic case shifted towards the smaller grain size.
Figure 5.5: Distribution of the number of neighboring grains for $N = 15000$. Square symbols (■) represent the isotropic case and the triangles (▲) and circles (●) represent the RS and ERS cases respectively.

Figure 5.6: Normalized frequency of normalized grain size distribution after simulation time step $=20000$ for isotropic case (■), RS grain boundary energy (▲) and ERS energy (●) cases.
Finally, the temporal variation of microstructural entropy (described by Bhadeshia and Sugden) \[102\], \( S = \sum \bar{A} \ln(\bar{A}) / \sum \bar{A} \); where \( \bar{A} = A_i / A_{ave} \) is the normalized area of \( i \)-th size group is calculated for the three cases. A plot of \( S \) with simulation time is shown in figure 5.7. This variation of entropies gives us information of size distribution profiles during evolution for the different mechanisms of grain growth. A smaller value of entropy (\( S \)) indicates that size distribution has narrow peak. The microstructural entropies of isotropic case (■) and RS anisotropic cases (▲) are not significantly different as observed in [35]. However, the ERS case (●) shows much higher microstructural entropy indicating broadening of the size distributions. This correlates with the observation of the grain structure in figure 5.2(c) showing the presence of a distribution of large and small grains. The ERS case shows that the system reaches a scaling regime and the microstructural entropy attains steady state for \( N > 30,000 \).

Figure 5.7: Evolution of microstructural entropy \( S \) with time. The isotropic (■) and anisotropic RS energy (▲) simulations show qualitatively similar evolution of the microstructural entropy. The ERS energy case (●) shows significantly faster broadening of the size distribution peaks.
5.6 Conclusions

We studied grain growth in isotropic and anisotropic systems. The anisotropic case was modeled using the Read-Shockley energy for low misorientation grain boundaries and an extended Read-Shockley energy with unrestricted misorientation. We used the active parameter tracking algorithm to efficiently simulate a large number of grains (each grain in the domain was assigned a unique orientation) with equiaxed orientation distribution. The grain growth rate in the system with ERS grain boundary energy was the lowest followed by the RS energy and the isotropic cases. Anisotropic ERS grain boundary energy shows the tendency to broaden the distribution of the grains to a bimodal distribution at later times.
CHAPTER – 6

Effect of second phase mobile and immobile particles on polycrystalline grain growth

6.1 Introduction

In a polycrystalline material, the grain size is a key microstructural length scale for mechanical and other physical properties. For example, reduction of the grain size gives better strength and toughness (Hall-Petch relationship [103]). Grain growth is a result of grain boundary migration to facilitate reduction of grain boundary energy. Thus, a possible mechanism for controlling grain growth is the reduction of grain boundary motion. Second phase particles exert a strong pinning effect (Zener pinning) on the grain boundary and provide a means of control of the microstructure.

This chapter presents a two-dimensional model of polycrystalline grain growth controlled by monodisperse mobile and immobile second phase particles. It is well known that the grain boundary mobility affects the microstructure and, thus, the overall mechanical and physical behaviour of polycrystalline materials. In turn, grain boundary mobility is strongly influenced by the presence of second phase particles. The aim of this study is to develop a phase field model for grain growth in a polycrystalline system in presence of monodisperse second phase mobile and immobile particles. As discussed before, the governing equations for microstructural evolution comprises a set of coupled non-linear partial differential equations (PDEs) of field variables, $\eta$.

The present model is an outgrowth of the phase field model of grain growth presented by Moelans et al [40], which was restricted to immobile particles only.
Moreover in their model the number of phase field variables was limited to thirty-six to represent the polycrystalline matrix. Our model is able to account for a large number of phase-field variables without associated burden on computational time or memory.

The grain boundary is pinned when the particles are immobile while particles are pushed by the grain boundary (driving force is proportional to the curvature of grain boundary) when particles are mobile. The interaction between grain boundary and the particles typically lead to a higher density for the mobile particles on the grain boundary than in the case of immobile particles [74].

6.2 Theory of particle pinning and dragging in a polycrystalline system

In a polycrystalline system, the grain growth is affected by those particles which are located on the grain boundaries only. In chapter 4, we discussed the driving force \( P_{gg} \) for grain boundary motion due to the curvature of the grain boundaries while the motion is opposed by pressure due to the presence of particles on the grain boundary. The grain boundary motion, i.e., the process of the grain growth ceases when the magnitude of both the forces (opposite in nature) is the same. However, the calculation of the drag force considered only a single particle. In fact, in a polycrystalline system each grain boundary may have more than one particle and hence the calculation needs to be revised. Let us consider a polycrystalline system where spherical particles of radius \( r_p \) with a volume fraction \( f_v \) are randomly distributed. The number of particles per unit volume \( n \) can be expressed as

\[
n = \frac{3f_v}{4\pi r_p^3}
\] (6.1)
For a planar boundary, the number of particles intersecting per unit area \( (n_s) \) of the grain boundary is

\[
n_s = 2r_p n = \frac{3f_v}{2\pi r_p^2}
\]

(6.2)

The total pinning force \( (P_z) \) arises from the particles on per unit area of the grain boundary is evaluated from equation (4.14) and (6.2)

\[
P_z = n_s P_{drag} = \frac{3f_v\gamma_b}{2r_p}.
\]

(6.3)

The term, \( P_z \) is known as the Zener pinning force [84]. The grain growth rate will stagnant for the following condition,

\[
\frac{dR}{dt} = m_b(P_{gg} - P_z) = 0, \quad \text{or} \quad \frac{c\gamma_b}{R} = \frac{3f_v\gamma_b}{2r_p},
\]

(6.4)

where \( R \) is the curvature of the grain boundary and \( c \) is the geometric constant of grain. If the mean grain radius is equal to the mean radius of the curvature then the limiting grain size yields

\[
R_z = \frac{2cr_p}{3f_v}.
\]

(6.5)

However, the above relationship is applicable only for the assumption of flat grain boundary interacting with a random distribution of particles where the particles at distance \( r \) behind the grain boundary contribute to the pinning force. The relationship for the limiting grain size \( (R_z) \) was being modified depending on the interaction mechanism [104], particles shape [105]. Haroun and Budworth [106] proposed the generalised form for the limiting grain size as
\[ R_z = \chi \frac{r_p}{f_v^b} \]  

(6.6)

The parameter \( \chi = 0.075 \) and \( b = 1 \) was considered for volume fraction \( f_v < 0.05 \) and \( \chi = 1.03 \) and \( b = 0.5 \) for \( f_v > 0.05 \).

The Zener relation in a two-dimensional system yields [107, 108]

\[ R_z = \frac{\pi r_p}{2 f_a} \]  

(6.7)

where \( f_a \) is the area fraction of the particles present in the system.

However, the particles may have its own mobility \( (m_p) \) and in this situation the grain boundary migration will continue along with particles (particle dragging by grain boundary) [72, 109]. The grain boundary will move with the particles if the driving force of grain boundary \( (P_{gg}) \) is lower than the pinning force \( (P_z) \) and the particles have its own mobility \( (m_p) \). In this situation, the velocity of grain boundary is given by

\[ v = \frac{m_p P_{gg}}{n_s} \]  

(6.8)

However, for larger value of \( P_{gg} (P_{gg} > P_z) \), the boundary leaves the particles and moves with a particle free motion. Figure 6.1 shows the grain boundary motion as a function of nondimensional driving force of the grain boundary.
6.3 Computational aspects

In this section, we apply our phase field model for grain growth in presence of mobile and immobile particles into a polycrystalline system. The model was initialised with randomly distributed particles of constant size in the entire domain of simulation area. We choose three different size of particles of radius $r_p = 2.5, 3.0$ and $4.0$. Figure 6.2 represents the discretized shape for particles of the above radius.

![Figure 6.1: Grain boundary motion as a function of the non-dimensional driving force.](image)

![Figure 6.2: Discretized geometry of the particles used in the simulations. The radius of particles are $r_p = 2.5, 3.0$ and $4.0$ from left to right.](image)

We start our simulation using the standard time dependent Ginzburg-Landau equation for the evolution of microstructure. As discussed previously, the polycrystalline
microstructure is described by the continuous field variables or the order parameters \( \eta_1(x,t), \eta_2(x,t), \ldots, \eta_Q(x,t) \), which are the function of material points \( x \) and time \( t \).

As mentioned in chapter five, at every grid point only few phase-field variables are active and contribute for the evolution of microstructure via grain boundary migration. To reduce the simulation time without adversely affecting the simulation results, we apply the active parameter-tracking (APT) algorithm. Thus, the equation (4.24) is modified and can be written as follows [38]:

\[
\frac{\partial \eta_{\xi_i}}{\partial t} = L_{\xi_i} \left( \kappa \nabla^2 \eta_{\xi_i} + \alpha \eta_{\xi_i}^2 - \beta \eta_{\xi_i}^3 - 2\eta_{\xi_i} \left( 2\nu \sum_{j=1}^{Q_a} \eta_{\xi_j}^2 - \sum_{k=1}^{Q_a} \eta_{\xi_k}^2 \right) \right), \quad (6.9)
\]

where \( \xi_i = 1, 2, \ldots, Q_a \) and \( \xi_i \leq Q \) at each simulation points. With this algorithm at every grid points, \( Q_a \) number of nonlinear equations are to be solved which is much smaller number than that of \( Q \) obtained from the classical algorithm. The details of this algorithm was discussed in chapter 5. For the evolution of \( \eta \), we solved the equation (6.9) in time and space. Particle movement and the prevention of interpenetration between particles are defined by the equation (4.25) and equation (4.26) respectively.

Considering an isotropic setting for grain growth, we use the value of gradient energy coefficient \( \kappa_i = \kappa = 2 \) and kinetic coefficient (related with mobility) \( L_i = L = 1 \) for all \( i \). The lattice step size and time step are chosen to be, respectively, \( \Delta x = 2.0, \Delta t = 0.25 \). Periodic boundary conditions are applied in both the \( x \)- and \( y \)- directions. Other phenomenological parameters, \( \alpha = \beta = \epsilon = 1 \) and \( \nu > \alpha/2 \) were taken in the entire simulation process. The additional phase field variable, \( \eta_k = 1 \) inside of the particle and
\( \eta_k = 0 \) in the matrix of the grain was considered. For the visualization of microstructure, we define a function

\[
\varphi(x, t) = \sum_{i=1}^{Q_a} \eta_{z_i}^2(x, t), \quad \xi_i = 1, 2, \ldots Q_a(x, t). \tag{6.9}
\]

whose values are 1.0 inside of the grain matrix representing white and significantly smaller positive values across the grain boundaries displayed as dark gray-level. The value of \( \varphi(x, t) > 1 \), indicating particles appeared as dark black spot. The sum is taken over the neighbouring active parameters. The area fractions of particles are taken to 1 to 15 percent of the total area of grains present. We compare the effect of number of particles, area fraction (with same number of particles) of particles and the mobilities of particles on the growth process. In the present simulation with the limitation of memory requirements of computer, we consider the domain sizes of 256\( \times \)256, 512\( \times \)512 and 1012\( \times \)1012 grid points. The details of the mathematical formulation and the procedure of numerical simulation are as discussed in chapter 4 and chapter 5.

### 6.4 Simulation results

In this section we present our simulation results for two-dimensional microstructural evolution of grain growth in presence of second phase mobile and immobile particles. Also, we present some results of single-phase grain growth for comparison.

Figure 6.3 shows the contours of \( \varphi(x, t) \) of evolving microstructure for particle free evolution (first row), evolution in presence of mobile particles (second row) and evolution in presence of immobile particles (third row) at simulation time steps \( N = 500, 12000 \) and 24000. The particle size \( r_p = 3.0 \) was considered for both mobile and immobile case. Total number of particle, \( p = 100 \) was taken. From the contours, it is clear that the
presence of immobile particles slows the grain evolution significantly whereas the mobile particles slows grain growth to a lesser extent. Particles are located on the grain boundaries after a few time steps. It has also been observed that in the evolution process, the growth is not homogeneous in presence of immobile particles and a crowd of small grains are located where most of the particles are present. This is because grain boundaries are arrested by the particles while boundaries move freely away from the particles. In the kinetics of grain growth in presence of mobile particles, the particles are dragged by the grain boundary and moved along with grain boundary. In this situation, the growths are more uniform in comparison with that of the immobile case. Mobile particles also show a tendency of congregation. The presence of immobile particles adversely effect on the grain growth process as compared to the presence of mobile particles with same volume fraction.
Figure 6.3: Simulation results for two-dimensional grain growth of a particle free (NP), in presence of mobile particles (MP) and immobile particles (IM) polycrystalline system in 512×512 system at time steps (a) $N = 500$; (b) $N = 12000$; (c) $N = 24000$. Total number of particles, $p = 100$ and the size of particle, $r_p = 3.0$. 
Figure 6.4 shows grain boundary pinning by immobile particles. In the initial microstructure, a few particles are observed inside the grain matrix which are marked by blue circle. As the evolution process continues, grain boundaries are pinned by the particles as shown in figure 6.4(b). In general after pinning, unpinning is rare as boundaries have a tendency to become straight and hence the driving force for the grain growth is reduced. However, the boundaries may detach from the particles if the driving force of grain boundary is increased and able to overcome the pinning force of the particles (Figure 6.4(c)). This was more clearly observed in the bicrystal case discussed in Chapter 4. Detachment from particles is not observed in presence of mobile particles. Particle will move with the grain boundary and do not become unpinned especially at higher mobilities of the particles [110].

Figure 6.4: GB pinning and sweeping during evolution in the presence of immobile particles. (a) initial microstructure where few particles are located inside the grains (blue circle), (b) almost all particles are on the GB after $N = 10000$ (c) GB detachment from the particles (red square) after $N = 25000$. Particle size $r_p = 2.5$ and total number of particle $P = 200$. 
We calculate the average grain diameter using \( D_{\text{ave}} = \frac{4A_{\text{ave}}}{\pi} \) where \( A_{\text{ave}} \) is the average area of grains calculated from the total area of the domain divided by the number of grains. The area of grain boundary is negligible compared to grain matrix and is hence ignored in the calculation of average area. Figure 6.5 shows the effect of particle size on the growth kinetics in the presence of mobile particles. The total number of particles was taken to be \( p = 100 \) with mobility coefficient, \( M = 50 \). Particle sizes of \( r_p = 2.5, 3.0, 3.5 \) and 4.0 was considered in 512×512 domain. It has been observed that for identical mobility and number of particles, the growth rate is inversely related to the particle size. As discussed before, the particle mobility strongly influenced by the particle size \([72]\) and hence the overall grain growth rate.

![Figure 6.5: The effect of particle size on the average diameter of grain as a function of simulation time. Total number of particles \( p = 100 \) and the mobility coefficient \( M = 50 \).](image-url)
Figure 6.6 shows the effect of mobility coefficient on the average grain size measured by the average diameter as a function of simulation time. The number of particles and particle size are taken to be $p = 100$ and $r_p = 3$ respectively. Results are also compared with particle free evolution and evolution in presence of immobile particles with same size and numbers that used in mobile case. Higher growth rate is observed in particle free evolution and followed by evolution in presence of mobile and immobile particles respectively. Furthermore, the growth rate strongly depends on the coefficient of mobility and faster growth was observed with higher mobility coefficient. The mobility coefficient in general depends on the nature of atomic diffusion (in the bulk or surface), atomic volume, absolute temperature and bulk diffusion constant [72].

![Figure 6.6: The effect of the mobility of the particles on the average diameter of grains as a function of simulation time. The size of particle, $r_p = 3.0$ and the total number of particles is $p = 100$.](image-url)
Figure 6.7 illustrates the effect of area fraction ($f_a$) of immobile particles on grain growth in a two-dimensional setting of 1024×1024 system. As the area fraction of immobile particles is increased, the growth rate slows down. For identical particle size, the grain growth is arrested earliest when $f_a$ is 7.0% of the grain matrix and followed by 3.5% and 1.0%. In consequence, the growth rates not only depend on $f_a$ but also depend on the size of the particles. For the same $f_a$, lower growth rate are observed in evolution with smaller particles and the growth ceased at lower mean grain size. This is not surprising because when the particle size is small, more particles are present for same $f_a$. As a result, more particles are on the grain boundaries which adversely effect on the grain boundary movement. A similar observation was observed by Ma et al in their cellular automata model [111].

![Graph showing the effect of area fraction ($f_a$) of immobile particles on average radius in a 1024×1024 system.](image-url)

Figure 6.7: Effect of area fraction ($f_a$) of immobile particles on average radius in a 1024×1024 system.
Figure 6.8 presents the ratio of average arrested grain radius to particle radius as function of area fraction ($f_a$) of monodisperse second phase immobile particles. We consider a system size of $1024\times1024$ for this case. From the Zener relationship of pinning pressure offered by the second phase particles, the mean final grain size ($R_Z$) (before cessation of growth) can be expressed by $R_Z = \chi r / f_v^b$, where $f_v$ is volume fraction, $r_p$ is the radius of particle, $b$ and $\chi$ are coefficients. The value of $\chi = 4/3$ and $b = 1$ gives for the maximum critical grain size in three-dimensional setting. However, the accurate description of the values of coefficients is controversial and many attempts are being made to improve the Zener relationship [112-114]. For high volume fraction of particle, most of the particles are located on the grain boundaries while for low volume fraction, particles are located randomly on grain boundary as well as inside of the grain matrix. The value of $\chi = 1.8$ and $b = 0.33$ for high volume fraction and $\chi = 0.222$ and $b = 0.93$ for low volume fraction was proposed by Hillert [115]. The Monte Carlo (MC) two-dimensional simulation results predicts the coefficients, $\chi = 1.73$ and $b = 0.5$ [108] or $\chi = 1.2$ and $b = 0.55$ [116] while front tracking 2D result gives $b = 0.5$ [117] or $b = 0.46$ [118]. For low area fraction of particles, the value of $\chi = 1.3$ was estimated by Fan et al [119] with an assumption of $b = 0.5$. Very recently, in two-dimensional phase field simulation, when all particles are located on the grain boundaries, the relationship between final mean radius ($R_Z$), particle radius ($r_p$) and the area fraction ($f_a$) of particle was predicted by Moelans et al [40] as $R_Z = 1.28 r_p / f_a^{0.5}$. From the linear fit of $\log(R_Z / r_p)$ vs. $\log(1/f_a)$ plot (not shown here) we calculate the value of coefficients $\chi = 1.18$ and $b = 0.48$ which gives a very good agreement with results given in [40, 117-119].
The temporal evolution of normalized grain size distribution in presence of second phase *mobile* particles and *immobile* particles are compared with the distribution of particle free evolution in figure 6.9. The simulation domain size was considered as $512 \times 512$ system. The distribution was counted after 20000 time steps. In isotropic grain boundary energy, the normalized grain size distribution for a single-phase system is expected to be constant in time. Our results of grain size distribution for particle free evolution confirms this. However, the peak of normalised grain size shifted towards the smaller grain size when particles are present and it is more pronounced for immobile case than that of the mobile one. The similar observation was observed by Hillert [1] and Abbruzzese [120] as predicted by the mean field theory. Due to the pinning tendency of

![Figure 6.8: Maximum average limited grain radius divided by particles radius as a function of area fraction of immobile particle during evolution of grain growth.](image)

For Immobile particles

$R_{Z/r_p}$

- $r = 2.5$
- $r = 3$
- $r = 4$
grain boundary by the particles, the grain growth is ceased before the significant modification of grain size distribution.

![Comparison of the distribution of normalized grain size for particle free evolution and evolution in presence of mobile and immobile particles after N = 20000. Particle size is $r_p = 3.0$, number of particles is $p = 100$ and the mobility coefficient is $M = 50$ in the simulations.](image)

6.5 Summary and concluding remarks

We extend our own numerical phase field model (discussed details in chapter 4 and chapter 5) for 2D polycrystalline grain growth in presence of mobile and immobile particles. The ability of APT algorithm reduced the computational requirements and successfully enables us to consider large number of order parameters. As the particles are not evolving in our simulation, their distribution was described by an order parameter
which is not evolved using the Ginzburg Landau equations. The effect of particle size and particle mobility are on growth processes have been considered. The increase of the area fraction of particles (either increasing particle size or increase of the number of particles) retards grain growth while increase of mobility accelerates grain growth process. The attraction force between particles and grain boundary is proportional to the size of particles. The kinetics of grain growth is affected by mobile and immobile particles and is approximated by a power law: $< R^m - R_0^m >= kt$, where the value of growth exponent, $m$ is greater than 2.0 (for ideal isotropic grain boundary energy with particle free case $m$ is equal to 2.0 [121]) and depends upon the particle size, particle mobility and volume fractions. The final mean grain size in presence of immobile particles (particles are present during the nucleation of grains and assumed all particles lie on the grain boundary) is expressed by Zener type relation $R_Z = \chi r_p / f_a^b$ with coefficients $\chi = 1.18$ and $b = 0.48$. This effect is much more pronounced in the case of immobile particles and followed by mobile particles. If the particles precipitate after some growth of grains, a large number of particles are present inside the grain matrix even after long time. Since particles inside the grain matrix does not affect the growth process, grain growth rate observed to be higher and the onset of growth stagnation is less defined and the time before stagnation is longer [40]. The interaction between particles and grain boundary affect the distribution of normalised grain size and the peak shifts toward the smaller grain size. This is due to the pinning effect imposed by the particles on grain boundary and as a result the grain growth ceases before the significant modification of grain size distribution. The effect is more pronounced in presence of immobile particles than that of mobile particles. A similar trend for the normalised grain size distribution for a system
containing second phase particles of radius $r_p = 3.0$ with area fraction $f_a = 0.02$ was observed by Moelans et al. [40]. Thus, our present simulation result gives a very good agreement with the literature works.
CHAPTER – 7
Conclusions and future work

Grain size plays an important role in the mechanical and other physical properties of materials. Hence, understanding the grain growth behavior and its control is of prime importance for the materials scientist. We have developed a new theoretical and computational model for grain growth in a polycrystalline system.

To understand the importance of grain size and hence grain growth phenomena, we start our work by the investigation of grain size dependent mechanical properties of Mg alloy where the presence of second phase particles are also observed.

We describe the effect of grain boundary energy and the presence of finely monodisperse second phase mobile and immobile particles on grain growth. The phase field theory was adapted for this purpose. An efficient APT algorithm was used for the computations. This approach reduces computational effort for simulations involving a large number of order parameters used. Our model predicts microstructural evolution which is in qualitative agreement with the work available in literature. The experimental results indicate the importance of grain size on tensile properties especially at high temperatures.

7.1 Summary of the results

We first investigate grain size dependent mechanical properties of Mg-3%Al alloys. The bulk alloy was prepared by powder metallurgy technique. The grain size of the nanostructured, ultrafine and microcrystalline samples was estimated as 80 nm, 120 nm,
and 12 µm respectively. It has been observed that the tensile properties are strongly depending on the grain size as well as the test temperature. At room temperature, the reduction of grain size gives better overall tensile properties. However, at elevated temperature the reduction of strength with a non-monotonic failure strain was observed in fine-grained samples.

Next our analytical study of the effect of mobile second phase particles described the interaction of a columnar grain boundary and uniformly dispersed mobile particles in an axisymmetric setting. We observed that the presence of particles retards the grain boundary motion. The particles move with the grain boundary when $m_p > m_b$, while the grain boundary may detach from particles if $m_b > m_p$ and the driving force of grain boundary motion exceeds the critical attraction force. This situation is consistent with the analytical results of Gottstein [72].

In the numerical model of grain growth in presence of mobile particles, we develop the phase field model for interaction with mobile particles. An additional constitutive kinetic equation ($v_p = m_p\kappa$) for each particle describes the motion of particles. The curvature $\kappa$ of the grain boundary is expressed explicitly in terms of the phase field variables. Particle interpenetration was prevented by introducing a repulsive force between two particles.

A close examination in a bicrystal system using the phase field model shows that the kinetics of the grain boundary is affected by the particle. The growth rate of the circular grain depends on the size and area fraction of particles. The mobility of particle is inversely proportional to the size of particle and thus increase in size of the particles retards the growth kinetics. The grain boundary obtains a dimple-like shape when it
approaches or leaves the particle. The first case is due to the local attraction of grain boundary by the particle while the second one is due to three surface tensions (one boundary surface tension ($\gamma_b$) and others boundary/particle surface tension ($\gamma_{AP}$ and $\gamma_{BP}$)) dictating the equilibrium shape of the boundary near the particle. In a dense particle system it was observed that the grain boundary dragged the particle cloud and creates a clear particle-free band behind the grain boundary. Similar particle dragging by migrating grain boundary in a polycrystalline copper was observed experimentally by Ashby and Gentamore [43].

In polycrystalline simulations we begin with the effect of anisotropic grain boundary energy on grain growth. Our grain boundary energy anisotropy is not restricted to low misorientations unlike previous work. For the high angle grain boundaries, we used the extended Read-Shockley (ERS) grain boundary energy [50]. We find that the energy anisotropy has a profound affect on the growth rate, grain size distribution and the number of neighboring grains. The average radius of grains is found to be proportional to the simulation time and the relationship is predicted by a power law. However, the energy anisotropy in grain boundary delays the growth rate and it is more pronounced in the ERS grain boundary energy and followed by RS. The normalized grain size distribution in an energy anisotropy shifts toward the smaller grain size indicating that growth is not uniform. The distribution of number of neighbouring grains is broader in the anisotropic case. All the above observations are in very good agreement with the results from literature [9, 32, 35, 101].

In the polycrystalline system, even a small volume fraction of second phase particles delays grain growth and leads to significant change in the grain size distribution. This
change is more pronounced in presence of immobile particles than that of mobile particles. It was observed that in the presence of particles, the peak of normalized grain size shifted towards the smaller grain sizes at later simulation times. In particle free grain growth, the above distribution is essentially invariant with time. The immobile particle pinned the grain boundary while the grain boundary dragged mobile particle. In both the cases (either grain boundary pinning or particle dragging) the effect of particles is based on the amount of grain boundary reduced by those particles which are located on the grain boundary. This interaction mechanism is consistent with the theoretical studies on Zener pinning [40, 118] or particle dragging [72, 74]. For immobile particles, we established the relationship of average stagnant radius ($R_Z$) in terms of area fraction. Assuming all particles are on the grain boundary, the average stagnant radius is predicted by $R_Z = 1.18 r_p / f_a^{0.48}$. This is in close agreement with values in the literature.

The main merits of this work to the materials scientist are as follows:

- Our experimental result gives an direct evidence that the grain size, structure of microstructure and the presence of second phase particles has a strong effect on the mechanical properties and thus models of grain growth and its control are very important.

- The presence of second phase particles plays an important role in controlling the final average grain size. The immobile particles pinned the grain boundary and are more effective to control the final average grain size than mobile particles. Nevertheless, in some cases particularly in sintered material the presence of mobile particles cannot be ignored and thus the consideration of mobile particles in our model of grain growth enhances this understanding.
The evolution of grain growth is a result of the reduction of free energy. The energy anisotropy of grain boundary influenced significantly on grain growth exponent, number of neighboring grains, grain size distribution and more.

The grain growth in a polycrystalline system is affected due to the presence of mobile particles. However, the retardation of growth process is more pronounced in the presence of immobile particles than that of mobile ones. The growth kinetics in presence of particles depends on the particle size, volume fraction of particles and the mobility of particles.
7.2 Future work

In order to build additional physical realism into the model, theory and experiment, a number of extensions and enhancements immediately suggest themselves, to wit:

1. The particles, as considered in Chapter 4 and Chapter 6, do not evolve through any diffusional processes. However, the evolution of particles may also be important in many cases and the particle sizes do not remain constant. Particle evolution may be accounted for by using a conserved order parameter field to describe the particles and solving the Cahn-Hilliard equations which describe the evolution in this setting.

2. It should be possible, within the general framework outlined in Chapter 5, to establish a three-dimensional model of high angle grain boundary energy anisotropy without restriction of the number of order parameters taken in simulation.

3. This work focused purely on the microstructural evolution aspects. It is possible to incorporate the effect of microstructure on the mechanical response. This is potentially an important extension of this work.

4. Grain growth in nanocrystalline materials occurs not only by the migration of the grain boundary but also by the coalescence of grains as a result of grain rotation [122]. Consideration of grain rotation could be one important extension of this work.
References


