2004

Mesoscopic simulation of abnormal grain growth

Rakesh Kumar Behera
Louisiana State University and Agricultural and Mechanical College

Follow this and additional works at: https://digitalcommons.lsu.edu/gradschool_theses

Part of the Mechanical Engineering Commons

Recommended Citation
https://digitalcommons.lsu.edu/gradschool_theses/1371

This Thesis is brought to you for free and open access by the Graduate School at LSU Digital Commons. It has been accepted for inclusion in LSU Master's Theses by an authorized graduate school editor of LSU Digital Commons. For more information, please contact gradetd@lsu.edu.
MESOSCOPIC SIMULATION OF ABNORMAL GRAIN GROWTH

A Thesis

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

in

The Department of Mechanical Engineering

by

Rakesh Kumar Behera
B.E., Regional Engineering College, Durgapur, India, 2000
August 2004
DEDICATION

This thesis is dedicated to my mother, Pramila Behera; my father, Biswanath Behera; my sisters, Bijay Laxmi and Bhagya Laxmi; my brothers, Rajesh and Rupesh; my brother-in-law, Sangram Keshari Nayak; Khusi Laxmi and Varsha Rath (Buturu).
ACKNOWLEDGEMENTS

I would like to express my sincere gratitude to Dr. Dorel Moldovan, my advisor, for his invaluable guidance and encouragement extended throughout the study. His tenacious supervision, helpful suggestion, patience and time deserve a special mention. I have learnt the basics of simulation under his guidance and would like to acknowledge his command in this area of research.

I would like to express my appreciation to my committee members Dr. E.I. Meletis and Dr. A. Raman for their support and suggestions. Thanks are extended to Dr. A. Raman for honing my fundamentals in Physical Metallurgy and to Dr. E.I. Meletis for teaching me the experimental techniques used in Materials Science.

I would like to thank my friends Dnyanesh Anaspure, Tushar Apshankar, Madhusmita Banerjee, Somo Banerjee, Nagaraj, Priya David, Kandra Deepak, Arvind Dwarapureddy, Vijay Gorugantu, Dr. Nikhil Gupta, Pankaj Gupta, Diwakar Iyer, Hemant Kathode, Harish Kingre, Phani Mylavarapu, Sunil Pal, Dinesh Pinnisetty, Sudheer Rani, Kanishk Rastogi, Rahul Maharsia, Rajeev Madazhy, Saurav Pathak, Biswamitra Patro, Varshni Singh, Dr. Vikram Singh, Sumit Singhal, Vikrant Thakare, Sridhar Thirumala, Shirin Vakil, Shengyu Wang, etc. for their constant help and valuable suggestions throughout the study. Special thanks are given to my students in the ME 3701-002 Lab.

I would like to express my gratitude towards my family members and relatives whose encouragement and support has been a constant source of inspiration during my stay at LSU.

Last, but not the least, I would like to gratefully acknowledge Louisiana Board of Regents for supporting the project.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEDICATION</td>
<td>ii</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>xi</td>
</tr>
<tr>
<td>1 INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 General</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Objectives</td>
<td>2</td>
</tr>
<tr>
<td>2 BACKGROUND AND LITERATURE REVIEW</td>
<td>4</td>
</tr>
<tr>
<td>2.1 General Review of Grain Growth Phenomena</td>
<td>4</td>
</tr>
<tr>
<td>2.1.1 Recovery</td>
<td>5</td>
</tr>
<tr>
<td>2.1.2 Recrystallization</td>
<td>5</td>
</tr>
<tr>
<td>2.1.3 Grain Growth</td>
<td>6</td>
</tr>
<tr>
<td>2.2 Normal Grain Growth</td>
<td>7</td>
</tr>
<tr>
<td>2.3 Abnormal Grain Growth</td>
<td>9</td>
</tr>
<tr>
<td>2.4 Theoretical Investigations of Abnormal Grain Growth</td>
<td>10</td>
</tr>
<tr>
<td>2.4.1 Factors Influencing Abnormal Grain Growth</td>
<td>10</td>
</tr>
<tr>
<td>2.5 Models for Grain Growth Simulation</td>
<td>13</td>
</tr>
<tr>
<td>2.5.1 Monte Carlo Potts Model</td>
<td>14</td>
</tr>
<tr>
<td>2.5.1.1 Potts Modeling Methodology</td>
<td>16</td>
</tr>
<tr>
<td>2.5.1.2 Applications of the Potts Model</td>
<td>19</td>
</tr>
<tr>
<td>2.5.1.3 Capabilities and Limitations of the Potts Model</td>
<td>19</td>
</tr>
<tr>
<td>2.5.2 Vertex Model</td>
<td>20</td>
</tr>
<tr>
<td>2.5.2.1 Vertex Modeling Methodology</td>
<td>21</td>
</tr>
<tr>
<td>2.5.2.2 Applications of Vertex Model</td>
<td>23</td>
</tr>
<tr>
<td>2.5.2.3 Capabilities and Limitations of Vertex Model</td>
<td>23</td>
</tr>
<tr>
<td>2.6 Comparison of the Two Modeling Methodologies</td>
<td>24</td>
</tr>
<tr>
<td>3 SIMULATION METHODOLOGY</td>
<td>26</td>
</tr>
<tr>
<td>3.1 Mesoscopic Simulation Approach</td>
<td>26</td>
</tr>
<tr>
<td>3.2 Simulation Model</td>
<td>27</td>
</tr>
<tr>
<td>3.2.1 Grain Boundary Properties</td>
<td>27</td>
</tr>
<tr>
<td>3.2.1.1 Grain Boundary Energy</td>
<td>27</td>
</tr>
<tr>
<td>3.2.1.2 Grain Boundary Mobility</td>
<td>29</td>
</tr>
<tr>
<td>3.2.2 Variational Formulation for Dissipative Power</td>
<td>31</td>
</tr>
<tr>
<td>3.3 Topological Changes</td>
<td>41</td>
</tr>
<tr>
<td>3.3.1 T1 Switch</td>
<td>41</td>
</tr>
</tbody>
</table>
LIST OF TABLES

4.1 Simulation results for area ratio value showing abnormal – normal transition. 74
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Typical recrystallization kinetics during isothermal annealing</td>
<td>6</td>
</tr>
<tr>
<td>2.2</td>
<td>Schematic representation of grain size distribution during normal grain growth</td>
<td>7</td>
</tr>
<tr>
<td>2.3</td>
<td>Temperature dependences of $n$ for isothermal grain growth in a variety of materials</td>
<td>8</td>
</tr>
<tr>
<td>2.4</td>
<td>Annealing of a severely deformed Al-3%Mg alloy with 0.5µm grains annealed at 250°C, shows normal grain growth</td>
<td>8</td>
</tr>
<tr>
<td>2.5</td>
<td>Schematic representation of grain size distribution during abnormal grain growth</td>
<td>9</td>
</tr>
<tr>
<td>2.6</td>
<td>Schematic representation of an idealized cellular microstructure, where the grains are approximated to hexagons of side $R$ and $\overline{R}$</td>
<td>11</td>
</tr>
<tr>
<td>2.7</td>
<td>Schematic of the basis of Monte Carlo simulation</td>
<td>15</td>
</tr>
<tr>
<td>2.8</td>
<td>Schematic flow chart of the Potts model</td>
<td>17</td>
</tr>
<tr>
<td>2.9</td>
<td>Schematic representation of 2D grain structure in a network model</td>
<td>21</td>
</tr>
<tr>
<td>3.1</td>
<td>Variations in energy ($\gamma$) and mobility ($m$) of a GB between two grains as functions of the misorientation angle $\theta$ for $\langle 001 \rangle$ tilt GBs, normalized using corresponding maximum values $\gamma_{\text{max}}$ and $m_{\text{max}}$ respectively</td>
<td>31</td>
</tr>
<tr>
<td>3.2</td>
<td>Schematic representation of velocity components on a single segment</td>
<td>33</td>
</tr>
<tr>
<td>3.3</td>
<td>Schematic representation of discretizing grain boundaries</td>
<td>39</td>
</tr>
<tr>
<td>3.4</td>
<td>Schematic representation of the velocity components acting on a moving segment</td>
<td>39</td>
</tr>
<tr>
<td>3.5</td>
<td>Schematic representation of T1 neighbor switching event</td>
<td>41</td>
</tr>
<tr>
<td>3.6</td>
<td>Schematic representation of T2 switching event</td>
<td>42</td>
</tr>
<tr>
<td>3.7</td>
<td>Schematic representation of T3 switching event</td>
<td>43</td>
</tr>
<tr>
<td>4.1</td>
<td>Four snapshots of a microstructure evolving by normal grain growth when (a) 10000, (b) 4724, (c) 2000, (d) 1030 grains are present</td>
<td>44</td>
</tr>
</tbody>
</table>
4.2 Size Distribution Plot for uniform microstructure

4.3 Time variation of average grain area during the growth of a uniform microstructure

4.4 Evolving microstructure in the presence of initially large grain with a geometrical bias of $R_b/<R> = 7.5$. Four snapshots are shown when (a) 10000, (b) 5443, (c) 1946 and (d) 1021 grains are present

4.5 Time evolution of $R_b/<R>$ with initial geometrical inhomogeniety

4.6 Time variation of average grain area with initial geometrical inhomogeniety

4.7 Time evolution of $R_b/<R>$ with mobility bias

4.8 Abnormal growth in the presence of GB mobility bias of $M_b/M = 7.0$ around a grain located close to the center of the simulation cell. Four snapshots are shown when (a) 10000, (b) 4995, (c) 2009 and (d) 1012 grains are present

4.9 Time variation of average grain area with grain boundary mobility bias

4.10 Time evolution of $R_b/<R>$ with energy bias

4.11 Abnormal growth in the presence of GB energy bias of $\gamma_b/\gamma = 0.4$ around a grain located close to the center of the simulation cell. Four snapshots are shown when (a) 10000, (b) 5212, (c) 2161 and (d) 1312 grains are present

4.12 Time variation of average grain area with grain boundary energy bias

4.13 Growth process in presence of 99 initial mobility biased grain with $M_b/M = 7$. Six snapshots are shown when (a) 10000, (b) 5168, (c) 2019 and (d) 1167, (e) 633 and (f) 181 grains are present

4.14 Time evolution of $R_b/<R>$ with mobility bias of 7.0 for 99 initial biased grains

4.15 Time variation of average grain area with 99 initial mobility biased grains
4.16 Growth process in presence of 250 initial mobility biased grain with $M_b/M=7$. Six snapshots are shown when (a) 10000, (b) 4890, (c) 1949 and (d) 1109, (e) 691 and (f) 125 grains are present.......................... 63

4.17 Time evolution of $R_b/<R>$ with mobility bias of 7.0 for 250 initial biased grains.................................................... 63

4.18 Time variation of average grain area with 250 initial mobility biased grains..................................................... 64

4.19 Growth process in presence of 500 initial mobility biased grain with $M_b/M=7$. Six snapshots are shown when (a) 10000, (b) 4938, (c) 2045 and (d) 1039, (e) 557 and (f) 156 grains are present.......................... 65

4.20 Time evolution of $R_b/<R>$ with mobility bias of 7.0 for 500 initial biased grains.................................................... 66

4.21 Time variation of average grain area with 500 initial mobility biased grains..................................................... 67

4.22 Growth mode in presence of 1000 initial mobility biased grain with $M_b/M=7$. Six snapshots are shown when (a) 10000, (b) 4952, (c) 2055 and (d) 1024, (e) 466 and (f) 157 grains are present.......................... 68

4.23 Time evolution of $R_b/<R>$ with mobility bias of 7.0 for 1000 initial biased grains.................................................... 69

4.24 Time variation of average grain area with 1000 initial mobility biased grains..................................................... 70

4.25 The grain size distribution plot in the presence of 1000 initial biased grains..................................................... 71

4.26 Radius ratio plot with respect to $% N_b/N_t$........................................... 72

4.27 Radius ratio plot with respect to $% A_b/A_t$........................................... 73

4.28 Microstructure evolution in and around the transition point in the presence of 99 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 4978, (b) 3512, (c) 2266, (d) 1726, (e) 1167 and (f) 633 grains are present................................................ 75

ix
4.29 Microstructure evolution in and around the transition point in the presence of 250 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 7747, (b) 5439, (c) 3768, (d) 1949, (e) 1109 and (f) 691 grains are present.

4.30 Microstructure evolution in and around the transition point in the presence of 500 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 7558, (b) 6436, (c) 4589, (d) 2930, (e) 1554 and (f) 1039 grains are present.

4.31 Microstructure evolution in and around the transition point in the presence of 1000 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 7992, (b) 5390, (c) 4952, (d) 4032, (e) 3525 and (f) 2559 grains are present.
ABSTRACT

Grain growth is the process that takes place during annealing of polycrystalline materials; its major feature is a systematic increase in grain size. Two different types of grain growth can be distinguished: the normal and abnormal grain growth. During normal grain growth, the microstructure exhibits a uniform increase in grain size with time and the grain size distribution follows the log-normal distribution with the grain sizes ranging from 0 – 2.2 times the average grain size (<R>). On the contrary, when the abnormal grain growth is the dominant mechanism, there are certain grains (abnormal grains) in the microstructure that grow much faster than the majority of the grains and in the end consume the fine-grained matrix around them. There has been a lot of work done in the field of abnormal grain growth, but the actual mechanism of abnormal grain formation and development from a uniform grain size distribution is not fully understood. In this study, various aspects of abnormal grain growth are investigated using a mesoscopic simulation approach.

Our investigation focuses on two possible venues that are, in general, considered as main sources promoting abnormal grain growth. The role of both the geometrical inhomogeneities (size effect) and grain boundary (GB) anisotropic properties are investigated. Simulations are done on various microstructures in which there are certain fraction of preexistent large grains (size greater than 2.2< R>), as well as on microstructures in which a given fraction of grains has different GB properties (mobility and energy). Our simulation results indicate that the presence of some large grains in the initial microstructure does not promote the abnormal grain growth. However, when certain grains in the microstructure have grain boundary energies below a certain
threshold or mobilities above a certain threshold value relative to the rest of the grains, the microstructure may evolve by abnormal grain growth.
1. INTRODUCTION

1.1. General

Grain growth is the process that takes place during annealing of polycrystalline materials and it has been an active topic of research over the last several decades. The significance of this process comes from the profound influences of the grain size and grain size distribution on a wide range of properties of polycrystalline materials. Grain size and grain size distribution are key parameters in sintered ceramic, metal, and alloy microstructures and have to be controlled during thermomechanical processing in order to ensure optimal mechanical properties.

Two different types of grain growth are known to develop during annealing; these are known as normal and abnormal grain growth [1]. During normal grain growth, the microstructure exhibits a uniform increase in grain size with time and the grain size distribution follows the log-normal distribution with the grain sizes ranging from 0 – 2.2 times the average grain size (\(<R>\)). On the contrary when abnormal grain growth is the dominant mechanism, there are certain grains (abnormal grains) in the microstructure that grow much faster than the majority of the grains and in the end consume the fine-grained matrix around them. The current work focuses on the issues concerning abnormal grain growth.

Abnormal grain growth has been studied for many material systems. Nanocrystalline nickel [2], electroplated copper [3], silicon steel [4], Ag thin films [5], Al-1wt % Mn alloy [6], Alumina doped with TiO₂ and SiO₂ [7], BaTiO₃ with 0.2 mol % excess TiO₂ [8], hard ferrite [9], etc. are the common systems studied for investigating abnormal grain growth. There are two stages characterizing the abnormal grain growth: the nucleation
and the growth stage. Due to the fast appearance and rapid growth of nuclei during abnormal grain growth, most of the studies focus on the growth stage only [9].

The presence of abnormal growth in an annealed microstructure has strong effect on the properties of the materials. It has been reported that annealing of nanocrystalline Ni reduces the strength many times due to abnormal grain growth [10]. In hard ferrites, used for permanent magnets, pore entrapment inside grains due to abnormal grain growth affects the coercive force. On the contrary, for systems like, sintered bismuth titanate powder and sintered alumina, abnormal grain growth is observed to be useful. Moreover abnormal growth mode can be used to obtain microstructure texturing due to grain alignment [9]. Therefore, it is important to establish the factors and conditions that promote the abnormal grain growth. A proper understanding will allow one to avoid, control or enhance the growth mechanism.

A lot of work has been done in the field of abnormal grain growth, but the actual mechanism of abnormal grain formation from a uniform grain size distribution is not fully understood. Rapid growth of the grains causes difficulties in capturing all the details during experimental observations. Therefore, computer simulations emerge as suitable tools to study the growth mechanism. The present study focuses on the different aspects of abnormal grain growth by using a mesoscopic simulation approach [11-12].

1.2. Objectives

The objectives of the present study are:

1. to determine the effect of the following factors on abnormal grain growth:

   (a) Geometrical Inhomogeniety (Size Bias)

   (b) Grain Boundary Mobility Bias
(c) Grain Boundary Energy Bias

2. to capture the abnormal – normal transition during abnormal grain growth.
2. BACKGROUND AND LITERATURE REVIEW

2.1. General Review of Grain Growth Phenomena

Grain growth is a common phenomenon, in polycrystalline materials, observed during high temperature treatment. Most of the properties, especially mechanical properties, of the materials depend on the grain size. For example, a small grain size distribution in the microstructure is required for materials with structural application at lower temperatures. Similarly, a large grain size distribution is favorable for high temperature creep resistance of the materials [13]. Therefore, the basic understanding of the growth mechanism is necessary for controlling the microstructure and properties of metals and ceramics according to the required application.

Grain growth normally occurs during casting, vapor deposition, electro deposition or the annealing of (cold worked) materials. Out of all these methods the evolution of the microstructure is explained easily by a simple grain growth mechanism in the annealing of the cold worked materials. However, one can argue that the same explanations can be used to explain the microstructure evolution for rest of the methods where primary recrystallization does not precede grain growth [13].

Annealing is a special heat treatment method in which a material is subjected to elevated temperatures for a longer time period and then cooled slowly. The annealing process consists of a heating stage, a holding/soaking stage and a cooling stage. Generally, this process is carried out to relieve the internal stresses, to increase the ductility and to obtain a specific microstructure in a material [14]. Thus, a cold-worked material is changed back to a strain-free microstructure by the full annealing process.
This annealing process can be divided into three stages: recovery, recrystallization and grain growth.

2.1.1. Recovery

This is a low temperature process with no appreciable change in the microstructure of the polycrystalline material which occurs before the recrystallization stage. The internal stresses created due to the cold-working of the material are relieved during this stage. At any given annealing temperature, the residual stress removal rate is higher at the beginning and decreases as the time proceeds. After releasing all the internal stresses in the microstructure, the recovered material is still observed to contain some elastic deformation. This is caused by the crystalline orientation difference of the grains, restricting the total relaxation of the microstructure. As the annealing temperature is increased most of the internal stresses are found to be relaxed. A lot of studies have been done on this topic. A complete recovery of the microstructure and properties, before irradiation or quenching for materials, has been established. Overall, there is a little change in hardness or strength observed during the recovery stage.

2.1.2. Recrystallization

This is the second stage of annealing process which starts as the applied temperature surpasses the upper temperature of the recovery range. Minute crystals nucleate in the microstructure having the same composition and lattice structure as that of the original undeformed grains. These strain-free nucleation sites combine and grow thereby leading to the process of recrystallization. The plot between the percent of the material recrystallized and time of annealing at a constant annealing temperature follows the typical Avrami model of any process driven by nucleation and growth.
Fig. 2.1. Typical recrystallization kinetics during isothermal annealing [13].

The figure above shows an incubation period in which the strain-free nuclei formed reach a visible critical microscopic size. Since there is no simple way to recreate the distorted structure (cold-worked), the growth of the recrystallized embryos is irreversible. Visible recrystallization begins after the incubation period.

2.1.3. Grain Growth

Grain growth occurs after the completion of the primary recrystallization step during annealing. The structure formed after primary recrystallization is not stable as there is still a large amount of energy stored in the grain boundaries of the newly formed grains. The reduction of the energy stored in the material in the form of grain boundaries is the driving force for the grain growth process. This driving pressure is reported to be two orders of magnitude less than that for primary recrystallization and it is typically of the order of $\sim 10^{-2}$ MPa [13]. Grain growth can be divided into two types: normal grain growth and abnormal grain growth or secondary recrystallization.
2.2. Normal Grain Growth

Normal grain growth is a continuous process during which the microstructure grows uniformly with the grain size distribution following a log-normal plot. When the grain size is scaled with the average grain size, this distribution describes a self similar growth process and its shape is independent of time for the entire growth process.

Fig. 2.2. Schematic representation of grain size distribution during normal grain growth [13].

Neglecting the initial transient, the grain size distribution can be expressed in terms of the mean radius. The power law relationship of the mean radius with the annealing time can be used to study the grain growth kinetics. The parabolic growth law deduced by Burke et al. [15] can be given as \( \bar{R}^2 = c_2 t \), where \( \bar{R} \) is the mean grain size at time \( t \) and \( c_2 \) is a constant. In general, this can be written as \( \bar{R} = c_2 t^{\frac{1}{n}} \), where \( n \) is the grain growth exponent and generally its value is above 2. For the ideal grain growth case, the predicted value of \( n \) is equal to 2.
Fig. 2.3. Temperature dependences of $n$ for isothermal grain growth in a variety of materials [13].

Fig. 2.3 shows the temperature dependence of the grain growth exponent in different metal and alloy systems. This discrepancy from the theoretical value of 2 derived by Burke and Turnbull has been attributed to various causes, e.g., the dependence of boundary mobility with the boundary velocity, limiting grain size distribution, etc. [16].

Fig. 2.4. Annealing of a severely deformed Al-3%Mg alloy with 0.5µm grains annealed at 250°C, shows normal grain growth [13].
The study done by Hayes et al. (2002), referred in [13], on severely deformed Al-3%Mg alloy with 0.5µm grains, annealed at 250°C, shows normal grain growth with $n = 2.6$ (Fig. 2.4).

2.3. Abnormal Grain Growth

Abnormal grain growth is a discontinuous process, where a few grains grow much faster than the rest of the grains in the microstructure. Thus, during abnormal grain growth a bimodal grain size distribution is predicted. However, as annealing continues, the grain size distribution is expected to follow a normal grain size distribution with larger average grain size than the initial microstructure.

Fig. 2.5. Schematic representation of grain size distribution during abnormal grain growth [13].

Due to similarity in growth kinetics and microstructure evolution with primary recrystallization, abnormal grain growth is known as secondary recrystallization. Though the basic cause behind abnormal grain growth is the reduction of the total grain boundary energy, the microstructural inhomogeneity of individual grains are expected to enhance the growth process. The presence of second-phase particles and texture are reported to enhance abnormal grain growth.
2.4. Theoretical Investigations of Abnormal Grain Growth

The effect of second phase particles has been studied analytically [1, 17] and experimental results showing abnormal grain growth in the presence of second-phase particles have been reported by several authors [13]. But many alloys contain second-phase particles wherein abnormal grain growth is not noticed during annealing. Therefore, the necessary conditions for the initiation or prevention of abnormal grain growth are not fully understood.

The effect of texture on the growth mechanism has also been studied extensively. The presence of a single strong texture in the microstructure leading to abnormal growth in aluminum, copper, nickel and silicon iron has been demonstrated. These studies imply that the presence of texture causes a change in the grain boundary properties (grain boundary energy and mobility) of the biased grain than the other grains in the microstructure. More detailed study has been performed and reported [18-20].

Other studies on the growth mechanism [21-22] indicate that abnormal growth can be easier in case of thin films or sheets than in bulk materials. Therefore, surface effects can also be key factors to influence abnormal grain growth. Some studies on the growth process due to the presence of small strains in the microstructure have also been analyzed.

2.4.1 Factors Influencing Abnormal Grain Growth

The quest on “why some microstructures grow uniformly or continuously, while some others non-uniformly or discontinuously” has led researchers to perform a thorough investigation on the factors influencing the growth mechanism in materials [1,13]. This analysis is done for an idealized cellular microstructure, as shown in Fig. 2.6 [13]. A
mean field model is developed to analyze the influencing factors, where boundary migration dictates the growth process. The effect of grain boundary inclination on the grain boundary properties is also neglected.

Fig. 2.6. Schematic representation of an idealized cellular microstructure, where the grains are approximated to hexagons of side $R$ and $\bar{R}$ [13]

In Fig. 2.6, $R$ is grain size, $\theta$ is the misorientation angle, $\gamma$ is the grain boundary energy and $M$ is the grain boundary mobility of a particular cell. This cell is embedded in a matrix having $\bar{R}, \bar{\theta}, \bar{\gamma}$ and $\bar{M}$ for mean grain size, misorientation angle, grain boundary energy and grain boundary mobility respectively.

Considering a 3-D assembly of grains of mean radius $\bar{R}$, the expression for the boundary velocity can be expressed as [1]

$$\frac{dR}{dt} = MP = M \left( \frac{\bar{R}}{R} - \frac{\gamma}{R} \right)$$

(Eq. 2.1)

where, $P$ is the pressure applied on the boundary during growth and all the boundaries have equal energy. Similarly, the growth rate of the large grain (radius $R$) with respect to the matrix can be represented as [13]

$$\frac{d}{dt} \left( \frac{R}{\bar{R}} \right) = \frac{1}{\bar{R}^2} \left( \frac{\bar{R}}{dt} \frac{dR}{dt} - R \frac{dR}{dt} \right)$$

(Eq. 2.2)
For abnormal grain growth to occur the following condition is to be satisfied [23]

\[
\left(\frac{R}{\bar{R}} \frac{dR}{dt} - R \frac{d\bar{R}}{dt}\right) > 0
\]  
(Eq. 2.3)

This will enable the large grain to grow much faster than the rest of the grains in the matrix. The expression for the rate of growth of a uniform grain assembly is given as [1]:

\[
\frac{d\bar{R}}{dt} = \frac{M \bar{\gamma}}{4\bar{R}}
\]  
(Eq. 2.4)

Therefore, considering equations 2.1, 2.3 and 2.4, the condition for abnormal grain growth can be written as:

\[
M \bar{\gamma} - \frac{R M \gamma}{\bar{R}} - \frac{R \bar{M} \bar{\gamma}}{4\bar{R}} > 0
\]  
(Eq. 2.5)

or,

\[
4R\bar{R}M \bar{\gamma} - 4\bar{R}^2 M \gamma - R^2 \bar{M} \bar{\gamma} > 0
\]  
(Eq. 2.6)

Dividing the above expression by \(\bar{R}^2 \bar{M} \bar{\gamma}\), the condition reduces to

\[
4\left(\frac{R}{\bar{R}}\right)\left(\frac{M}{\bar{M}}\right) - 4\left(\frac{M}{\bar{M}}\right)\left(\frac{\gamma}{\bar{\gamma}}\right) - \left(\frac{R}{\bar{R}}\right)^2 > 0
\]  
(Eq. 2.7)

or,

\[
4XQ - 4QG - X^2 > 0
\]  
(Eq. 2.8)

where, \(X = \left(\frac{R}{\bar{R}}\right)\) = the grain size term

\(Q = \left(\frac{M}{\bar{M}}\right)\) = the grain boundary mobility term

and \(G = \left(\frac{\gamma}{\bar{\gamma}}\right)\) = the grain boundary energy term

The roots of the equation \(4XQ - 4QG - X^2 = 0\), defines the limits for normal / abnormal grain growth. Thus, from the above explanation it is clear that abnormal grain growth depends on the grain size, grain boundary energy and grain boundary mobility of a
particular grain with respect to the rest of the grains in the matrix. A thorough study of the effects of these individual factors is studied by performing mesoscopic simulation. Simulation results are explained in the Results and Discussion section of the thesis.

2.5 Models for Grain Growth Simulation

Grain growth is the process which takes place during the annealing of polycrystalline materials; the major feature is a systematic increase in grain size. To understand the growth mechanism a lot of work has already been done both experimentally and theoretically. However, there are still many important questions which are unanswered and the quest on the growth kinetics is the motivating factor for the ongoing researches and the current study too.

The theoretical study on grain growth dates back to more than 50 years. However the results of the studies were not fully supported by the experimental findings and therefore, a lot more theoretical models were developed in the last 30 years. In general, the theoretical approach to the grain growth study relies on a lot of simplifying assumptions and constraints and therefore computer simulation has generated a lot of interest among the researchers and has gained a lot of attention lately.

The modeling approaches can be broadly divided into two categories: micro models and coupled models. Micro models basically simulate individual processes e.g., annealing (recovery, recrystallization or grain growth), deformation, etc. Coupled models can simulate a combination of deformation and annealing, multi-pass hot-rolling, etc. Micro models are used in the current study and they can be classified in the following groups:
1. Monte Carlo Potts model \((10^{-9} \text{m}-10^{-5} \text{m})\) which can be used to study recrystallization and grain growth of the annealing process.

2. Kinetic Ginzburg-Landau Phase Field model \((10^{-9} \text{m}-10^{-5} \text{m})\); used in general to study polycrystal and polyphase grain coarsening, precipitation formation and coarsening.

3. Dislocation Dynamics model \((10^{-9} \text{m}-10^{-4} \text{m})\) used to study recovery and microtexture.

4. Geometrical, Topological and Component model \((10^{-7} \text{m}-10^{-2} \text{m})\). This model can be used to study recrystallization, grain growth and secondary recrystallization of the annealing process.

5. Vertex model \((10^{-7} \text{m}-10^{-2} \text{m})\), also known as Network model or Grain boundary Dynamics model. It is used in simulation studies of nucleation, recovery, subgrain coarsening, recrystallization, grain growth and secondary recrystallization.

6. Cellular Automata model \((10^{-9} \text{m}-10^{-5} \text{m})\); used in studies of recrystallization, grain growth and phase transformation phenomena.

Depending on the actual physical phenomena to be studied, one has to decide on the simulation model to be used, by carefully examining the constraints and limitations of the model. For grain growth studies, Monte Carlo Potts model and Vertex model seem to be the most promising and both models have been used widely by various researchers. In the next section we give a brief overview of these two simulation models.

2.5.1 Monte Carlo Potts Model

Monte Carlo (MC) Potts model is based on a probabilistic description of grain boundary migration [24-25] and is a common method used in studies of microstructural
evolution in polycrystalline materials. A variation of this model called the kinetic multistate Potts models was also developed by Anderson et al. [20, 25-26].

This model, proposed by Potts, is based on the general Ising model used for studies of the critical phase transitions in magnetic materials. Similar to the Ising model, Potts model is based on a discrete spin like representation of the system in which stable structures evolve by minimizing the boundary between the spin-up and spin-down domains. Basically in a Potts model the system is divided into a number of discrete points arranged on a regular lattice. Each point represents the centers of small areas or volumes of system. Within these regions the microstructure is assumed to be homogeneous. Each domain may have a characteristic state variable such as orientation, surface energy, lattice energy, dislocation density, etc. These extended domains with identical values of the characteristic state variables can be considered as grains in the polycrystalline materials.

![Fig. 2.7. Schematic of the basis of Monte Carlo simulation [13].](image)

Fig. 2.7 represents a microstructure where individual domains are differentiated from each other by the state variable called grain orientation. The grain boundaries limiting each grain are the regions in which there is a change of the state variable and characterize the interaction of the given grain with the surrounding ones (e.g., 4/3 or 4/6
or 4/7 or 4/2 or 4/9 type boundaries for domain with characteristic state variables value 4). Thus, the number pair of the state variable is the key parameter that is used to extract information about the moving boundaries during simulation. Moreover, grain boundary energies are specified in terms of the number pairs. For like number pairs a zero energy value is assigned and for unlike pairs a high energy value (e.g., one) is assigned.

2.5.1.1 Potts Modeling Methodology

The schematic flow chart for the simulation procedure of the Potts models is shown in Fig. 2.8 [25, 27]. The total energy of the system can be expressed as a function of orientation by a classical Potts-type Hamiltonian equation such as the one proposed by Anderson et al. [25, 28]

\[
E = J_{gb} \sum_i \sum_j \left( 1 - \delta_{S_i S_j} \right)
\]  
(Eq. 2.9)

where, \( J_{gb} \) is the scaling factor for grain boundary energy

\( S_i \) is the orientation of the domain considered

\( S_j \) is the orientation of the nearest neighbor site of the domain considered

\( \delta_{ij} \) is the Kronecker delta function

According to the equation 2.9, the total energy is calculated summing over all the sites \( i \) and over all the nearest neighbors (\( m \)) of site \( i \). The grain boundary energy (interfacial energy only) has a value of zero in the grain interior and arbitrary positive value, \( J_{gb} \), at grain boundary sites. Considering a more generalized Q-state Potts model, the exact value of the interfacial energy \( J_{gb} \) could vary.
Fig. 2.8. Schematic flow chart of the Potts model.
The grain growth phenomenon is simulated by searching for possible switches of all lattice sites to the value of one of the neighboring site. During a typical Monte Carlo switch trial, if the total energy of the system remains the same or decreases, the switch is favorable and it is acceptable. If the total energy of the system would increase after switching, then the transition of the lattice sites can be accepted with a certain probability. This transition probability can be expressed as \[ W = \begin{cases} \exp\left(\frac{-\Delta E}{k_B T}\right) & \text{if } \Delta E > 0 \\ 1 & \text{if } \Delta E \leq 0 \end{cases} \] (Eq. 2.10)

where, \( \Delta E \) is the change in the total energy of the system

\( k_B \) is the Boltzmann constant

And \( T \) is the temperature in Kelvin

A critical issue in MC Potts model simulations is the nature of the time. Basically in the simulation time is defined in terms of the total of Monte Carlo Step (MCS) and temperature. Various studies have been dedicated to derive the relationship between the three parameters. A simple relationship was given by Radhakrishnan et al. [28]:

\[ MCS = v \exp\left(-\frac{Q}{RT}\right) \cdot t \] (Eq. 2.11)

in which the MCS is proportional to the time \( (t) \). A more complex relationship was proposed by Gao et al. [29] and it is based on the grain boundary migration (GBM) model and reads:

\[ (MCS)^{2n} = \left(\frac{L_0}{K_1 \lambda}\right)^2 + 4\gamma AZv^2 \exp\left(\frac{\Delta S_i}{R}\right) \sum \exp\left(-\frac{Q}{RT_i}\right) \cdot t_i \] (Eq. 2.12)

where, \( v \) = the atomic vibration frequency

\( L_0 \) = the initial grain size
\( \lambda \) = lattice point spacing

\( \gamma \) = grain boundary energy

\( A \) = the accommodation probability

\( Z \) = the average number of atoms per unit area at the grain boundary

\( N_a \) = Avogadro’s number

\( h \) = Plank’s constant

\( \Delta S_f \) = the fusion entropy of the material

\( Q \) = molar activation energy

\( R \) = the gas constant

\( T_i \) = the temperature in time interval \( t_i \),

and \( K, K_1, n \) and \( n_1 \) are constants

Due to the ambiguities in defining the time, the classical Monte Carlo approach cannot simulate the kinetic details of the grain growth process.

### 2.5.1.2 Applications of the Potts Model

The Potts Model has been extensively used to simulate many materials phenomena, such as primary recrystallization [13, 30-35], secondary recrystallization [36-37], dynamic recrystallization [38-40], grain growth [25-29, 41] and texture evolution [42-44], etc.

### 2.5.1.3 Capabilities and Limitations of the Potts Model

The Potts model has the advantage of being very simple to code and simulate. Grain boundary energies and mobilities are the only parameters that are needed to simulate a simple growth process, e.g., grain growth in single phase materials. This model is capable of simulating in general larger systems in comparison to other methods.
Due to its simplicity, it can be used to simulate other physical phenomena such as thin film growth by molecular beam epitaxy [45].

The major drawback is its inability to simulate complex phenomena such as recrystallization, where a lot of assumptions and relationships between the system variables are needed as input into the model. The ambiguity in defining the time in a Potts model simulation is another major drawback. Also, it is very difficult, in general, to monitor the growth of any individual grain as the sampling site is selected randomly from the whole area during each calculation.

2.5.2 Vertex Model

Vertex model is another simulation methodology in which the explicit topological representation of the microstructure is used. The microstructure is represented by grain boundary segments interconnected through triple junctions. Therefore, the model deals with the grain boundary and triple junctions (vertexes), the periodic spatial distribution of which will represent the microstructure under study. The motion of grain boundaries and triple junctions is followed by time integration of their position assuming the normal velocity for the boundary to be proportional to the boundary curvature. Grain growth takes place due to the movement of the boundaries and the vertices. Therefore, the challenge for simulation remains in accurately determining the velocity and direction of the boundaries and vertexes during growth. There are two types of vertex models that are used in grain growth studies: in one of these models one calculates the motion of the boundary segments whereas in the other the vertex motion is calculated. The vertex model was pioneered by R.L. Fullman in 1952 and later on lot of variations have been proposed and implemented.
Fig. 2.9 represents a two-dimensional schematic representation of a typical grain structure in a network model [13]. At each simulation step, the nodal points $N_i$, the position of the vertexes and the corresponding neighbor lists are stored. Thus, this method is more economical in comparison to the Potts Model in terms of computing, where the state variables of all the sites in the simulated area are stored in each MCS.

2.5.2.1 Vertex Modeling Methodology

The basis of the theoretical and analytical approach in vertex model deals with the local curvature and the stored energy of the boundaries, as these are the driving forces for the motion of the boundary segments and vertexes during growth [46-47]. The velocity of a grain boundary segment ($v$) can be written as:

$$v = MP$$  \hspace{1cm} (Eq. 2.13)

where, $M$ = mobility of the boundary

$P$ = the driving force, which is proportional to the curvature of the boundary and the grain boundary energy.
The curvature of any grain segment is determined by the force balance at each vertex, the balance condition called Herring relation, which and can be expressed as:

\[
\frac{\gamma_{23}}{(1 + \varepsilon_2 \varepsilon_3) \sin \psi_1 + (\varepsilon_3 - \varepsilon_1) \cos \psi_1} = \frac{\gamma_{13}}{(1 + \varepsilon_1 \varepsilon_3) \sin \psi_2 + (\varepsilon_1 - \varepsilon_2) \cos \psi_2} = \frac{\gamma_{12}}{(1 + \varepsilon_1 \varepsilon_2) \sin \psi_3 + (\varepsilon_2 - \varepsilon_3) \cos \psi_3}
\]

(Eq. 2.14)

Here, \(\gamma_{ij}\) is the specific grain boundary energy between grains i and j, \(\varepsilon_i = \frac{\partial \ln \gamma_{(ii)}}{\partial \psi}\) is the torque term and is determined by the anisotropy of the grain boundaries. The expression for \(\varepsilon_i\) shows that the energy of the boundaries depend on the spatial orientation of the adjacent boundary planes \(\psi\). Using the well-known Read-Shockley equation, the grain boundary energy for low angle boundaries (misorientation less than 15°) is calculated. In general, for the rest of the grains with high angle boundaries (misorientation greater than 15°), the grain boundary energy is considered to be constant for simulation process.

In a 2D grain growth process, the motion of each node is subjected to the traction from all three boundaries connecting through the node. Therefore the total driving force acting on any node can be given by the addition of the individual forces,

\[
F_i = \sum_{j=1}^{3} F_j^i
\]

(Eq. 2.15)

where, \(F_i = \) driving force acting on node \(i\)

\(F_j^i = \) driving forces of the three boundaries linking the \(i\)th node and is given by

\[
F_j^i = \left(\frac{2\gamma_{ij}}{R_j}\right)\hat{n}_j
\]

(Eq. 2.16)

where, \(R_j = \) the radii of curvature of the three boundary segments
\[ n_j = \text{unit vector normal to the boundary surfaces} \]

The individual grain boundaries can be discretized further within two or more nodes to incorporate curvature to the boundaries. Topological changes are included to get rid of the much smaller segments during simulation. According to the Mullins-von Neumann law for 2D grain structures, the grain growth kinetics is related to the topological class of individual grains as (von Neuman 1952; Mullins 1956):

\[
\frac{dA}{dt} = k_N (N - 6) \tag{Eq. 2.17}
\]

where, \( A \) = grain area

\[ N = \text{topological class of the grain} \]

And \( k_N = \text{kinetic constant.} \)

According to the von Newman-Mullins relation, grains with the number of sides less than six are forced to shrink and may eventually disappear, whereas those with more than six sides will grow.

2.5.2.2 Applications of Vertex Model

The vertex model has been used to study the dynamics of the grain growth process quite successfully over the last two decades. In particular it proved to be very successful in simulation studies of microstructural evolution such as: nucleation and grain growth [46, 48-52] and recovery and recrystallization [47, 52-54].

2.5.2.3 Capabilities and Limitations of Vertex Model

As opposed to the Potts model the vertex model is capable of calculating the motion dynamics of each individual continuum defect entity (dislocation segment, boundary segment or vertex, etc.) directly. This model calculates the motion of the lattice defects, usually on the basis of capillary and elastic forces, unlike Potts model, where the
dynamics is obtained by minimizing the total energy of the system. This model gives the best visual effect for the simulated results. Moreover the time has the real physical meaning in a vertex simulation model.

The basic limitation of the vertex model is that this model does not consider the influence of the physical properties inside grains or subgrains on the microstructural evolution. This procedure cannot aptly treat the problem of dot nucleation and growth as the curvature approaches near infinity. Also, this model is very difficult to extend to 3D simulation due to the complexity of 3D topography.

2.6 Comparison of the Two Modeling Methodologies

The comparison of the two models can be given as follows:

1. Potts model is very simple and easy to program compared to the vertex model which require more coding effort.

2. Potts model is a stochastic model and automatically updates topological changes. On the contrary the vertex model is deterministic and necessary topological changes have to be accounted for by explicit programming in simulation code.

3. Simulating 3-D structures is relatively easy using Potts model but it is very difficult with the vertex model.

4. More assumptions and more relationships are needed for handling complex problems, like static and dynamic recrystallization, using Potts model. Vertex model is a better method for these conditions.

5. During annealing, growth occurs due to the migration of the grain boundaries. Potts model shows limitations in treating the grain boundaries. Vertex model is more efficient and reliable for simulating annealing condition.
Recent work by Radhakrishnan et al. [55] on curvature driven growth established doubt on the correct implementation of the Potts model. The investigation was based on the subtle difference between the type of flip probability (probability of flipping the boundary sites) function used during the simulation. The flip probabilities depend on the type of visit to the boundary sites during each time-step. As the implementation of the algorithm is not clear, the study indicates uncertainty in the already published results. Therefore, based on the accuracy, Vertex model is preferred over the Potts model for the current study. Mechanisms such as subgrain rotation and coalescence [56] can also be included in Vertex model.
3. SIMULATION METHODOLOGY

3.1 Mesoscopic Simulation Approach

Most of the systems that are present in nature are known to exist in the form of closed cells with well-defined boundaries, e.g. soap froths, biological tissues, lipid monolayers, etc. [57]. These cellular systems are the basis of modeling the initial arrangement of grains in a polycrystalline material. The grain boundaries, which contain excess energy, are represented by the cell walls. Considering a 2D model, the microstructure can be represented by grain boundaries and triple points. The process of grain growth is simulated by following in time the motion of the boundaries, motion driven by the reduction of the total energy of the system.

The theoretical approach for investigating the microstructural evolution in our mesoscale simulation study is based on a variational principle for dissipative systems [58]. This formalism was originally used for studies of grain boundaries and surface diffusion during void growth. Later, Cocks and Gill [59] and Gill and Cocks [60] adapted the variational functional for simulating curvature driven grain growth. Their modification of the variational functional describes the power (rate of energy) dissipation due to the competition between the reduction in grain boundary energy and the viscous drag proportional to the boundary velocity.

The equations for minimizing velocity fields are obtained by applying D’Alembert’s differential form of the variational principle. Recently Cleri [57] developed a stochastic formulation based on the Cocks - Gill formulation of the functional and he used it to study the 2D grain growth by Velocity Monte Carlo (VMC) simulation approach, in which the variational functional was used as a transition-rate generating
function. The simulation method is called VMC, as it samples random velocities rather than random displacements as in the Monte Carlo (MC) method. This approach can be used to study the growth mechanism with all possible factors affecting the energy dissipation, e.g., grain sliding, grain rotation [56, 61-62], matter diffusion along grain boundaries [63], etc.

3.2 Simulation Model

3.2.1 Grain Boundary Properties

Grain boundary energy and mobility are the two most important grain boundary properties. These play an important role during recovery, recrystallization and grain growth. Despite their importance GB properties are in general very difficult to measure experimentally as there are many variables which affect their properties. Therefore, a complete understanding of the grain boundary properties is yet to be established.

In general depending on their misorientation angle, $\theta$, grain boundaries can be classified as high angle grain boundaries ($\theta > 15^\circ$) and low angle grain boundaries ($\theta < 15^\circ$). Moreover experimental studies on polycrystalline materials show that the grain boundary properties are anisotropic and depend on the amount of misorientation $\theta$ across the grain boundary [13, 64].

3.2.1.1 Grain Boundary Energy

For a low angle grain boundary, the relationship between the grain boundary energy and misorientation is given by the well known Read and Shockley formula which was derived analytically using a dislocation model of the low angle grain boundary. This relationship reads:

$$\gamma_s = \gamma_0 \theta (A - \ln \theta)$$  \hspace{1cm} \text{(Eq. 3.1)}
where, $\theta = \text{misorientation angle given by } \theta \approx \frac{b}{h}$,

$b = \text{burgers vector magnitude of the grain boundary dislocation}$

$h = \text{spacing between adjacent dislocations in the boundary}$

$\gamma_s = \text{energy of the boundary}$

$\gamma_0 = \frac{Gb}{4\pi(1-\nu)}$

$A = 1 + \ln\left(\frac{b}{2\pi r_0}\right)$

$r_0 = \text{the radius of the dislocation core (usually between } b \text{ to } 5b\).$

It is evident from this relationship that the energy of the low angle boundary will increase with increase in the misorientation $\theta$. This leads to a decrease in the energy per dislocation. This relation is found to hold reasonably well up to $\theta \sim 15^\circ$ misorientations, above which the dislocations get closer and closer leading to an overlap of the dislocation cores and the model fails.

For the current mesoscopic simulation a modified Read-Shockley relationship introduced by Wolf [65], extended to large misorientation angles, has been considered. For $\langle 001 \rangle$ tilt boundaries this can be written as:

$$\gamma(\theta) = \sin(2\theta)\left(\frac{E_c}{b} - \frac{E_s}{b}\ln[\sin(2\theta)]\right)$$

(Eq. 3.2)

where, $E_c = \text{dislocation-core energy}$

$E_s = \text{strain-field energy}$

The above equation 3.2 can be normalized with respect to the maximum grain boundary energy ($\gamma_m$) and is given as:
\[ \frac{\gamma(\theta)}{\gamma_{\text{max}}} = \sin(2\theta)(1 - r \ln[\sin(2\theta)]) \]  

(Eq. 3.3)

where, \( \gamma_{\text{max}} = \frac{E_c}{b} \) and \( r = \frac{E_s}{E_c} \)

From the equation, the value of \( r \) will indicate how steeply the grain boundary energy curves rise at low angles. This also sets the range of misorientations over which a grain boundary may be considered as a low-angle grain boundary.

### 3.2.1.2 Grain Boundary Mobility

In general when there is a driving force (pressure for example) acting on a grain boundary this will migrate so as to reduce the total energy of the grain boundary network. It is generally assumed that the velocity (\( v \)) is directly proportional to the net pressure (\( P \)). The relationship can be written as:

\[ v = MP, \]  

(Eq. 3.4)

where \( M \) is the proportionality constant regarded as the mobility of the boundary. The mobility of the grain boundaries is temperature dependent. It can be represented by an Arrhenius type relationship as [12]:

\[ M = M_0 \exp\left( -\frac{Q}{RT} \right) \]  

(Eq. 3.5)

where, \( Q \) is the activation energy related to the atomic scale thermally-activated process which controls boundary migration. This can be obtained from the slope of the plot between \( \ln(M) \) and \( 1/T \).

Grain boundary migration involves diffusion in and across the boundary. Therefore, it is expected that the structure of the boundary (e.g. orientation relationship) will have some effect on the boundary mobility. It has been reported [66] that apart from
temperature, boundary misorientation ($\theta$) affects the mobility of the boundaries. For low angle boundaries ($\theta < 15^\circ$), increase in misorientaion results in higher dislocation density in the boundaries and decrease in mobility. The activation enthalpy for migration is observed to be close to self diffusion for $\theta < 10^\circ$. Therefore, boundary misorientation of these types of boundaries is found to have lower effect on mobility. The activation enthalpy for migration at higher $\theta$ is lower and is close to boundary diffusion. Winning et al. [67] showed that under stress the relative mobilities of high and low angle boundaries depend on temperature. The results for aluminum indicated that at high temperatures low angle boundaries move much faster than high angle boundaries. Similar study on curvature driven boundary migration [68] resulted in different mobility values for high angle boundaries which depend on the tilt axis.

For high angle grain boundaries ($\theta > 15^\circ$) the relationship between orientation and mobility is well established. The mobility of the high angle boundaries is higher than that of low angle boundaries. Studies performed on high purity bicrystals of aluminum and other metals [69] resulted in extensive mobility measurements during curvature driven grain growth.

For current simulation the grain boundary mobility is assumed to depend on misorientaion and independent of the grain boundary plane inclination. The relationship used was proposed by Humphreys and is given by

$$
\frac{m(\theta)}{m_{\text{max}}} = 1 - \exp \left[ -B \left( \frac{\theta}{\theta_0} \right)^n \right]
$$

(Eq. 3.6)
The variation of grain boundary properties with misorientation can be represented as in Fig 3.1.

3.2.2 Variational Formulation for Dissipative Power

The initial microstructure is generated by a Voronoi construction consisting of irregular interconnected polygons. Each side of the polygon between two triple junctions represents a grain boundary. Grain boundaries with more than three junctions are physically unstable, hence discarded if generated. Let the individual length of the grain boundaries be given by $L_i$, where $i = 1, 2, \ldots, N_{gb}$ with excess energy $\gamma_i$. $N_{gb}$ is the total number of grain boundaries generated in the Voronoi construction. Therefore, the total number of triple points generated can be given as $N_{tj} = (2/3)N_{gb}$. Similarly, the total number of grain boundaries can be given as $N_{gb} = 3N$, where $N$ is the total number of grains in the microstructure.
During the growth the grain boundaries can elongate or shrink or can move perpendicular away or towards their center of curvature (grain boundary migration) depending on whether or not this GB motion minimizes the local energy. Certain amount of energy is dissipated during the GB motion and the evolution will follow the path that is consistent with minimization of total power dissipated.

Considering the elongation or shrinkage of all of the boundaries, the system will evolve so as to reduce the excess interfacial energy, \( \sum_{i=1}^{N_{gb}} (\gamma_i L_i) \), by reducing the excess energy regions (i.e. the total grain boundary perimeter). The rate of work done can be written as

\[
W_T^* = \sum_{i=1}^{N_{gb}} \int_{L_i} \dot{\gamma}_i \dot{\epsilon}_s^*(s) \, ds
\]  
(Eq. 3.7)

where, \( \dot{\epsilon}_s^* = \frac{1}{\Delta t} \left( \frac{\Delta L_i^*}{\Delta L_i} \right) \)

and \( \dot{\epsilon}_s^* \) is known as the rate of change of virtual variation of the boundary length.

Similarly, considering the grain boundary migration for these boundaries, the rate of internal energy dissipation by the viscous force (\( f \)) is given by

\[
W_M^* = \sum_{i=1}^{N_{gb}} \int_{L_i} f \dot{v}_n^*(s) \, ds
\]  
(Eq. 3.8)

where, \( \dot{v}_n^* \) is a set of virtual velocities normal to the grain-boundaries, produced by the set of virtual \( \dot{\epsilon}_s^* \). A set of virtual velocities \( \dot{v}_s^* \) along the grain-boundaries is also produced.

We define the variational functional \( \Pi \) for the total dissipated power during the grain-
boundary migration and the above expressions for $W^*_T$ and $W^*_M$ are combined into a “virtual power principle” given as [57]:

$$\Pi[v(x)] = \sum_{i=1}^{N_{gb}} \left[ \gamma_i v_n(x) \kappa_i \, ds + \int_{L_i} \gamma_i \frac{\partial v_s(s)}{\partial s} \, ds + \int_{L_i} \frac{v^2_s(s)}{2 \mu_i} \, ds \right]$$

(Eq. 3.9)

where, $\gamma_i = \text{the excess energy}$; $\kappa_i = \text{curvature of the boundary}$; $\mu_i = \text{mobility}$; the length of the $i^{th}$ grain boundary is given as $0 \leq s \leq L_i$ and the grain boundary coordinates are denoted by the vector field $x$.

Assuming that the GBs can be represented approximately as a collection of straight segments (GB discretization representation) we derive next the detailed expression for the variational functional terms describing such a system. Consider that we know for a given GB segment both the coordinates of the end points $(x_1, y_1)$ and $(x_2, y_2)$ and the velocity of each node $\vec{v}$ ($v_x, v_y$). The velocity components along the segment can be determined by the velocities of the end points 1 and 2 (positive direction from 1 to 2).

![Fig. 3.2. Schematic representation of velocity components on a single segment](image)
The tangent unit vector (consistent with the positive direction chosen) is given by

$$\hat{s} = (s_x, s_y) = \frac{1}{d} (x_2 - x_1, y_2 - y_1), \text{ with } d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} \tag{Eq. 3.10}$$

The unit vector perpendicular to this will be \(\hat{n}\) satisfying \(\hat{n} \cdot \hat{s} = 0\) (also chose \(\hat{n} \perp \hat{s}\) with \(\hat{s} \times \hat{n} > 0\)). Assuming \(\hat{n} = (n_x, n_y)\):

$$\hat{n} \cdot \hat{s} = n_x s_x + n_y s_y = 0 \tag{Eq. 3.11}$$

or,

$$\frac{n_x}{n_y} = -\frac{s_y}{s_x} \tag{Eq. 3.12}$$

One way of satisfying this would be by

(1) \(n_x = -s_y\) and \(n_y = s_x\), which automatically satisfies \(\hat{s} \times \hat{n} > 0\)

Knowing \(\hat{s} \times \hat{n} = s_x n_y - s_y n_x > 0\), the choice given by (1) would do just fine. Therefore, the normal and tangent components of the velocity can be calculated. The normal component of velocity:

$$v_n = \vec{v} \cdot \hat{n} = v_x n_x + v_y n_y$$

$$= -v_x s_y + v_y s_x \tag{Eq. 3.13}$$

or,

$$v_n = -v_x \left(\frac{y_2 - y_1}{d}\right) + v_y \left(\frac{x_2 - x_1}{d}\right) \tag{Eq. 3.14}$$

Similarly, the tangent component of velocity:

$$v_s = \vec{v} \cdot \hat{s} = v_x s_x + v_y s_y \tag{Eq. 3.15}$$

or,

$$v_s = v_x \left(\frac{x_2 - x_1}{d}\right) + v_y \left(\frac{y_2 - y_1}{d}\right) \tag{Eq. 3.16}$$

Thus the variational functional can be written as

$$\Pi[v(x)] = \sum_{i=1}^{N_n} \left[ \gamma_i v_n(x) \kappa_i \, ds + \gamma_i (v_{i1} \cdot s_{i1} + v_{i2} \cdot s_{i2}) + \int_{L_i} \frac{v_n^2(s)}{2\mu_i} \, ds \right] \tag{Eq. 3.17}$$
The variational functional shown in equation 3.17 contains three terms corresponding to the dissipative processes by a motion of a GB segment [59]. The first term (curvature term) is a contribution due to the grain-boundary curvature. This expression indicates that the curvature driven boundaries will move at a rate directly proportional to the local curvature and $\gamma_i$. The second term (grain-boundary energy term) corresponds to the contribution due to the tangent displacement of the triple points. The term shows that the sum of the scalar products of the velocity and the tangent vector at the end-points of each grain boundary is the net force acted in moving the triple points. The last term (grain-boundary mobility term) shows the energy dissipated due to the viscous force opposing the migration perpendicular to the boundary.

The total variational functional $\Pi[v(x)]$ given by Eq. 3.17 can be made stationary by a set of variational parameters $\tilde{v}(x)$ (velocities of triple junctions). This can be given as:

$$\delta \Pi[v(x)] = 0 \quad for \ v(x) = \tilde{v}(x)$$

(Eq. 3.18)

This velocity field can be used to obtain the new network configuration, e.g., by a forward time-integration. If the boundary configuration changes from $\alpha$ to $\beta$, then the kinetic evolution can be obtained from the following expression:

$$X(\beta) = X(\alpha) + \tilde{v}(x) \cdot \Delta t$$

(Eq. 3.19)

where, $\tilde{v}(x)$ is the velocity field minimizing the functional. Such an evolution is associated with a minimal energy change given by

$$\Delta H_{\alpha\beta} = \Pi[\tilde{v}(x)] \Delta t$$

(Eq. 3.20)

Minimizing the variational functional can be approached in two ways [57]. One way is to use the discretized representation of the grain-boundary network, which will
lead to replacement of the continuous velocity field by a set of velocities of some discrete nodal points. The second approach involves the introduction of some shape functions describing local curvature along grain boundaries. This will help in integrating the curvature term, thus leaving only the triple-junction velocities as the variational parameters [59]. Both approaches require the writing of the variational functional $\Pi$ as a function of a discrete set of velocities $\{v_i\}_{i=1,2,\ldots,M}$. Minimization of this functional can be done using a global (Finite element) method or by using approximate local (Monte Carlo) method. A typical system of interest has a very large number of degrees of freedom due in part to the thousands of grains that have to be present in a system. Moreover, the minimization procedure has to be repeated many times in order to predict the time evolution of the microstructure. The simulation of such a fully coupled solution of the equations of motion for many grain boundaries for long times is a cumbersome process and it is also costly in terms of computation resources even with the fastest computers available today. Thus, the local Monte Carlo method (where the trial variations are performed on one random variable at any time), specifically the VMC method is used. Computationally, this method scales linearly with the system size, and it requires the calculation of the energy differences rather than the nodal forces. In this method a stochastic description of grain growth based on the derived variational formulation is used. The result of grain boundary migration (growth) is turned into a random sequence of microscopic configurations. Basically, the velocity Monte Carlo algorithm is implemented as follows:

Considering two microscopic configurations $\alpha$ and $\beta$, the probability per unit time of the change in configuration from $\alpha$ to $\beta$ can be given as:
where $W = \text{transition probability}$. The transition probability can also be written in terms of energy dissipation rate as:

$$W(\alpha \rightarrow \beta) = \begin{cases} \frac{1}{\tau} \exp\left( -\frac{\Delta \Pi(v_k \cdot \Delta t)}{\kappa T} \right) & \text{if } \Delta \Pi(v_k) > 0 \\ \frac{1}{\tau} & \text{if } \Delta \Pi(v_k) \leq 0 \end{cases} \quad \text{(Eq. 3.22)}$$

where, $\tau$ is a normalizing factor obtained as the sum of the waiting times for all allowed transitions and $T$ is a fictitious temperature related to the amplitude of random contribution. During each Monte Carlo step the velocity is varied randomly as: $v'_k = v_k + \chi v_k$, where $\chi$ is a random number, uniformly distributed between -1 and 1. This is sampled for each triple junction $k$. The variational functional $\Pi$ is calculated for two cases:

(i) with $v_k$ equal to the velocity from the previous time step

(ii) with $v_k$ equal to a randomly variational velocity $v'_k$

The varied velocity $v'_k$ is accepted if

(i) the value of the dissipated power decreases, $\Pi(v'_k) < \Pi(v_k)$
in case of \( \Pi(v_k) > 0 \), if the Boltzmann-Metropolis test results in
\[
\xi < \exp\left( -\frac{\Delta \Pi(v_k) \cdot \Delta t}{K_B T} \right),
\]
where \( \xi \) is a random number uniformly distributed between 0 and 1.

Otherwise, the old value of \( v_k \) is kept. Thus, at each subsequent time step, the position of the triple junction \( k \) will be updated by using
\[
X_k(\beta) = X_k(\alpha) + v^*_k(x) \cdot \Delta t,
\]
(Eq. 3.23)

where \( v^*_k \) can be either \( v_k \) or \( v'_k \) according to the accepted calculated velocity. So, \( v^*_k \) is the velocity field corresponding to \( \delta \Pi[\nu(x)] = 0 \).

The absolute value of \( W \) is governed by the scaling parameter \( k_B T \). The parameter \( v_k \) in the expression for \( W \) represents the velocity fields of the two configurations \( \alpha \) and \( \beta \), which differs only for the velocity of the \( k^{th} \) triple junction and the three boundaries that share the triple junction. Thus, the variational formulation is reduced to a stochastic sequence of elementary changes. These changes correspond to individual, uncorrelated grain boundary migrations. Therefore, the unknown velocity field \( v_k \) in equation 3.22 is a set of random variables sampled during the simulation with an equilibrium distribution represented by \( W \). Within thermodynamic limit, it is shown that the time dependent average quantities computed with such a stochastic sequence converge to the deterministic approach [57].

For the present study the equations used for the VMC simulation method can be generated with the basic variational formulation (equation 3.17). The grain boundaries generated with a Voronoi construction is discretized to provide curvature to the grain
boundaries as normally observed in the microstructure of polycrystalline samples. Thus, each segment is considered to be straight with zero curvature (Fig. 3.3).

**Fig. 3.3. Schematic representation of discretizing grain boundaries.**

For each grain boundary segment the curvature term in the variational functional is eliminated. Thus,

\[ \Pi[v(x)] = \sum_{i=1}^{GR_{segm}} \left[ \gamma_i \left( \nu_i \cdot s_{i1} + \nu_{i2} \cdot s_{i2} \right) + \int \frac{\nu_n^2(s)}{2 \mu_i} ds \right] \]  
(Eq. 3.24)

**Fig. 3.4. Schematic representation of the velocity components acting on a moving segment**
Let us consider the $i^{th}$ element as shown in Fig. 3.4. For the segment, the first term of $\Pi$ represents the contribution of the reduction of the excess energy. This can be given by $\gamma_i (\vec{v}_{i_1} \cdot \vec{s}_{i_1} + \vec{v}_{i_2} \cdot \vec{s}_{i_2}) = \gamma (v_{s_2} - v_{s_1})$.

The second term represents the normal component of velocity. Assuming that at the end of the straight boundary the normal components of the velocities are $v_{n_1}$ and $v_{n_2}$, the variation of $v_n$ along the grain boundary will be:

$$v_n(s) = \vec{v}(s) \cdot \hat{n} = v_{n_1} + z(v_{n_2} - v_{n_1}), \text{ where } 0 \leq z \leq 1$$

(Eq. 3.25)

Therefore, the second term (mobility term) can be expressed as

$$\int_{L_i} \frac{v_n^2}{2\mu_i} ds = \frac{L_i}{2\mu_i} \int_0^1 v_n^2(z) dz$$

$$= \frac{L_i}{2\mu_i} \left[ v_{n_1}^2 + z^2(v_{n_2} - v_{n_1})^2 + 2zv_{n_1}(v_{n_2} - v_{n_1}) \right] dz$$

(Eq. 3.26)

$$= \frac{L_i}{2\mu_i} \left[ v_{n_1}^2 + \frac{1}{3}(v_{n_2} - v_{n_1})^2 + v_{n_1}(v_{n_2} - v_{n_1}) \right]$$

$$= \frac{L_i}{6\mu_i} \left[ (v_{n_1})^2 + (v_{n_2})^2 + (v_{n_1})(v_{n_2}) \right]$$

Thus, the equation for the $i^{th}$ segment can be represented as

$$\Pi_i(\vec{v}_{i_1}, \vec{v}_{i_2}) = \gamma_i (\vec{v}_{i_1} \cdot \vec{s}_{i_1} + \vec{v}_{i_2} \cdot \vec{s}_{i_2}) + \frac{L_i}{6\mu_i} \left[ (v_{n_1})^2 + (v_{n_2})^2 + (v_{n_1})(v_{n_2}) \right]$$

(Eq. 3.27)

The total expression for the variation functional is obtained by integrating the above expression over the total grain boundary segments. The final expression is given as follows:

$$\Pi(\{\vec{r}\}, \{v\}) = \sum_{i=1}^{GB\ segms} \left[ \gamma_i (\vec{v}_{i_1} \cdot \vec{s}_{i_1} + \vec{v}_{i_2} \cdot \vec{s}_{i_2}) + \frac{L_i}{6\mu_i} \left[ (v_{n_1})^2 + (v_{n_2})^2 + (v_{n_1})(v_{n_2}) \right] \right]$$

(Eq. 3.28)
After each VMC step, the node positions \( \{r\} \) of the field is updated by a simple forward integration based on the new node velocities as \( r_i(t+dt) = r_i(t) + v_i dt \).

### 3.3. Topological Changes

During grain growth the average grain diameter and grain area increases. This happens as some grains grow while others shrink and eventually disappear. Thus, the topology of the system evolves continuously. During the evolution of the microstructure certain vertices may be driven closer and closer to each other and therefore appropriate actions must be incorporated into the simulation algorithm to account for possible discrete topological changes. In one of the first simulation studies on time evolution of cells structures, Weaire and Kermode [70] have defined three such basic topological transformations. One can also show that the whole range of topological changes occurring in an evolving microstructure can be obtained from a finite combination of the following discrete topological events:

#### 3.3.1. T1 Switch

T1 switch, also known as neighbor-switch, occurs when a grain boundary becomes shorter than some fraction \( \Delta_{T1} \) of the scaled characteristic length in the system. In our system the value of \( \Delta_{T1} \) is taken as 2% of the scaled characteristic length. The schematic representation of a T1 switch is shown in Fig. 3.5.

![Fig. 3.5. Schematic representation of T1 neighbor switching event](image-url)
The figure indicates that the nodes C and D come much closer to each other and the grain boundary length (\(\Delta\)) falls within the critical length defined in the simulation. Prior to T1 switch grains A and B were the neighbors. After T1 switch, grains C and D become neighbors with a slight increase in the grain boundary length \([\Delta(1+\varepsilon)]\) between nodes A and B. The transformation can be visualized as a continuous process with an intermediate state represented by the middle figure, which is physically unstable.

3.3.2. T2 Switch

T2 switch, also known as three-sided cell disappearance event, occurs when the area of a grain becomes smaller than some fraction \(\Delta_{T2}\) of the scaled characteristic area in the system. The grain is observed to be three-sided and is removed from the network during the switch. The schematic representation is given below (Fig. 3.6).

![Fig. 3.6. Schematic representation of T2 switching event](image_url)

In the above representation the area of grain A becomes smaller than the scaled characteristic area in the system. Thus, grain A is removed and a new triple junction is created with grains B, C and D. In our system the value of \(\Delta_{T2}\) is taken as 0.1% of the scaled characteristic area.
3.3.3. T3 Switch

T3 switch, also known as two-sided cell disappearance event, takes place when a two-sided cell consisting of only two triple junctions is formed due to a T1 or T2 switch. The figure shown below represents how a T2 switch generates a two-sided grain. A T3 switch is followed restoring a stable microstructure.

Fig. 3.7. Schematic representation of T3 switching event
4. RESULTS AND DISCUSSION

The current study is performed with mesoscopic simulation approach. Before using the method for studying abnormal grain growth, it is necessary to verify the accuracy by studying the well established facts for grain growth. It is well known that microstructures containing uniform grain size distribution with uniform GB properties will lead to normal grain growth during annealing. The result of our simulation for normal grain size distribution and uniform GB properties supports normal grain growth. Fig. 4.1 shows four snapshots with approximately 10000, 5000, 2000 and 1000 grains left in the microstructure. The visual inspection qualitatively indicates that normal grain size distribution is maintained during the time evolution of the system.

![Fig. 4.1. Four snapshots of a microstructure evolving by normal grain growth when (a) 10000, (b) 4724, (c) 2000, (d) 1030 grains are present.](image-url)
It is known that the average grain size $\langle R \rangle$ is a valid scaling parameter. This reduces the grain size distribution function $f(x) = f(\frac{R}{\langle R \rangle})$ at different times to a common curve. Fig. 4.2 shows the variation of the normalized distribution function for the above case. The function for the initial Voronoi structure (10000 grains) shows a narrow peak around $x = \frac{R}{\langle R \rangle} \approx 1$ and a relatively symmetrical normal distribution. As growth continues, the peak height of the distribution gradually decreases and the width broadens until the scaling regime is reached. During growth, the distributions were calculated when 8000, 6000 and 3000 grains were left in the system. A typical normal grain growth plot is obtained for each case, indicating that the growth is taking place normally.

Fig. 4.2. Grain Size Distribution Plot for uniform microstructure
The time evolution of the average grain area is another indicator of the nature of growth. According to growth law, \( A(t) \propto t^n \), where \( n \) is known as the grain-growth exponent and is determined by taking the linear regression fit to the linear portion of the \( \log[A(t)] \) vs. \( \log(t) \) curve. Our simulation result shows (Fig. 4.3) a linear increase of the mean grain area with time (i.e. \( n \approx 1.0 \)). This matches with already reported exponent value for normal grain growth [11, 52, 60].

![Graph showing the time variation of average grain area during the growth of a uniform microstructure.](image)

**Fig. 4.3.** Time variation of average grain area during the growth of a uniform microstructure.

The above qualitative and quantitative analysis indicates that the current model satisfactorily predicts the well known facts regarding normal grain growth. Therefore, the same model can be used to study abnormal grain growth.
4.1 Possible Causes for Abnormal Grain Growth

During synthesis of polycrystalline materials, abnormal grains can be observed in the microstructure. As discussed in the earlier chapter (3.4.1) there are three possible venues that can be considered as main sources promoting abnormal grain growth [71]. Either the preexistence of already large grains (size greater than 2.2<\(R\)) in the original microstructure or difference in the grain boundary (GB) mobility and GB energy surrounding certain grains (which may be due to the presence of some coarsening particles or texture), can promote abnormal grain growth. Each of these possible mechanisms is investigated in this study by simply tracking the time evolution of a single grain whose initial size and local environment (its GB properties) are varied in a controlled manner.

The simulations are done for the three possible factors in which an arbitrary grain located close to the center of the simulation cell has: (a) an initial geometrical bias, (b) GB mobility bias, that is, all the surrounding GBs have mobilities larger than the average and (c) GB energy bias, in which the surrounding GBs have energies smaller than the average. The condition for abnormal grain growth is assessed by monitoring the time evolution of the relative size \(R_b/<R>\), where \(R_b\) is the radius of the tagged grain and \(<R>\) is the average radius of the rest of the grains in the matrix for each of the three cases. Each simulation is performed with 10000 initial grains and the triple-point equilibrium condition is not enforced a priori. Therefore, the initial structure relaxes over a few MC steps and the data are analyzed soon after the Herring relation is recovered in the simulation.
4.1.1 Initial Geometric Inhomogeneities (Grain Size Effect)

This study is done with the preexistence of an already large grain (size greater than 2.2\(<R>\)) in the original microstructure with uniform GB properties. There may be two possibilities. (a) The large grain in the microstructure may grow faster due to size bias resulting in abnormal grain growth, or (b) the size effect will have no substantial influence and the grain will grow normally due to uniform GB property. The study is conducted over a range of size bias (S = R_b/<R>) in the initial microstructure with R_b/<R> nearly 2.5, 5.0, 7.5, 10 and 15. Results analyzed for all the cases indicate that the presence of large grains with uniform GB properties in the microstructure will always lead to normal grain growth.

![Evolving microstructure in the presence of initially large grain with a geometrical bias of R_b/<R> =7.5. Four snapshots are shown when (a) 10000, (b) 5443, (c) 1946 and (d) 1021 grains are present.](image-url)
The explanation is given for a typical simulation run with the initial size of the “tagged” grain ($R_b/\langle R \rangle$) about 7.5 times larger than the average grain size. Fig. 4.4 shows four snapshots similar to the normal grain growth study. The visual inspection indicates that during microstructure evolution the growth rate of the tagged grain is slower than the growth rate of the rest of the grains in the matrix. Thus, the size advantage present initially for the tagged grain is gradually lost in time. Therefore, the microstructure approaches the typical microstructure of normal grain growth. To support the visual inspection, the time evolution of the relative size of the tagged grain is monitored with respect to $\langle R \rangle$. Fig. 4.5 shows the plot between $R_b/\langle R \rangle$ and simulation time.

![Graph showing time evolution of $R_b/\langle R \rangle$](image)

**Fig. 4.5. Time evolution of $R_b/\langle R \rangle$ with initial geometrical inhomogeneity**

**NOTE:** The values written besides each curve (e.g. 2.5, 5.0,..) indicates size bias of the tagged grain with the initial Voronoi construction. The data is analyzed after the Herring relationship is recovered. Therefore, the $R_b/\langle R \rangle$ values do not match the initial ratio for the corresponding runs.
The radius ratio curves have a negative slope for all the cases studied. This indicates that the size of the tagged grain decreases with time, approaching the average grain size of the rest of the grains in the system. If the simulation is done for a large system, it is expected that the tagged grain will eventually be no different from the rest of the grains (in terms of the size) in the microstructure. Thus, for the ideal case the ratio $R_b/<R>$ will reach a value close to 1.0. Each curve shows a faster drop during the initial period of the growth process, followed by a slower drop towards the end of the simulation. This suggests that the system with the initial size bias is thermodynamically unstable during annealing and reaches a more normal configuration as soon as possible.

The comparison of the later stages of the plots shows that the curves are almost parallel to each other. This predicts that the growth rates for all the cases are equivalent.

![Graph showing time variation of average grain area with initial geometrical inhomogeneity.](image)

**Fig. 4.6.** Time variation of average grain area with initial geometrical inhomogeneity.
The nature of evolution with initial geometrical inhomogeneity is further analyzed by the growth law. The results are then compared with the known case of normal grain growth. Fig. 4.6 represents that the growth plot with initial size bias follows the plot for normal grain growth with a growth exponent $n \sim 1.0$. Therefore, the simulation results show that the preexistence of a large grain in the microstructure with uniform grain-boundary properties does not promote abnormal grain growth. The influence of size bias is obtained to support the already published results [23, 25, 72-74]. The rest of the study will focus on the effect of grain boundary properties on the grain growth phenomena.

4.1.2 Grain Boundary Mobility Bias

It is well known that the velocity of a grain boundary is directly proportional to its mobility. Therefore, grain boundaries with higher mobilities move faster than those with lower mobilities during annealing. The effect of mobility is studied by biasing the GB mobilities of all the GBs surrounding the “tagged” grain, an arbitrary grain located close to the center of the simulation cell. The mobility ratio $m = M_b/M$ ($M_b$ is the mobility of GBs surrounding the tagged grain and $M$ is the mobility of all the other GBs) of 2.0, 2.3, 3.0, 5.0, 7.0, 10.0, etc., are considered for this study.

It is interesting to note that the plot between $R_b/\langle R \rangle$ and simulation time (Fig. 4.7) show that for some mobility biases the curve have a negative slope while for others a positive slope exits. Normal grain growth is observed for the conditions which result in a negative slope. On the other hand, abnormal grain growth is promoted for conditions which result in a positive slope. This implies that there exists a threshold which guides the behavior of grain growth. At threshold, the radius ratio value is maintained throughout the simulation and the curve is parallel to the time axis. This critical value for
a normal grain size distribution with mobility bias only is observed to be around $M_b/M=2.3$ (Fig. 4.7).

![Graph showing time evolution of $R_b/<R>$ with mobility bias](image)

**Fig. 4.7. Time evolution of $R_b/<R>$ with mobility bias**

Simulation results indicate that above the critical mobility bias the slope of the individual plots increases with increase in the mobility bias. Thus, the biased grain grows much faster than the rest of the grains in the matrix. This preferential growth due to mobility bias dictates abnormal grain growth in the system. The supporting evidence for abnormal grain growth is presented for a mobility bias ($M_b/M$) of 7.0. The snapshots shown in Fig. 4.8 clearly indicate that the biased grain grows rapidly at the expense of the rest of the grains in the system. Though the initial microstructure shows a uniform grain size distribution, mobility bias of the grain boundaries has a pronounced effect on the nature of growth during annealing.
Fig. 4.8. Abnormal growth in the presence of GB mobility bias of \( M_b/M = 7.0 \) around a grain located close to the center of the simulation cell. Four snapshots are shown when (a) 10000, (b) 4995, (c) 2009 and (d) 1012 grains are present.

Further analysis is done by obtaining the grain growth exponent for the case of \( M_b/M = 7 \). The results are then compared with the known case of normal grain growth. Fig. 4.9 represents that both the growth plots follow each other for a certain initial period of time, after which the mobility bias plot shows a sharp upward rise. The grain growth exponent for the mobility bias case is found to be nearly 1.2, which is greater than the exponent for normal grain growth (\( n = 1.0 \)). Thus, the simulation results show that the preexistence of mobility bias in certain boundaries with uniform grain size distribution will promote abnormal grain growth.
Fig. 4.9. Time variation of average grain area with grain boundary mobility bias.

Similar studies have been performed for the other important grain boundary property - grain boundary energy. Its effect on the nature of growth is reported in the following section.

4.1.3 Grain Boundary Energy Bias

It is well known that boundaries with lower energy can bend, curve and stretch easily. Thus, it is expected that grain boundaries with lower energy can enhance the easy migration of the boundaries leading to abnormal grain growth. Results are obtained for the case when only grain boundary energy bias $\gamma_b/\gamma$ is present ($\gamma_b$ is the energy of GBs surrounding the tagged grain while $\gamma$ is the energy of all the other GBs). The GB energy values ($\gamma_b/\gamma$) considered for the current study are 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3 and 0.2.
The results obtained with the time evolution of the radius ratio plot indicate that for certain energy bias values the curve shows a negative slope, while for certain cases it shows a positive slope. Abnormal grain growth is observed for the energy bias values for which the curve results in a positive slope. Fig. 4.10 shows that abnormal growth is observed for most of the lower energy cases. Similar to the mobility bias case, a threshold is obtained. The critical value for GB energy bias is observed to be around $\gamma_b/\gamma = 0.8$. Below this critical value, abnormal grain growth proceeds.

![Graph showing time evolution of $R_b/\langle R \rangle$ with energy bias](image)

**Fig. 4.10. Time evolution of $R_b/\langle R \rangle$ with energy bias**

The microstructural evolution due to energy bias showing abnormal grain growth is presented in Fig. 4.11 for a particular case of $\gamma_b/\gamma = 0.4$. The initial microstructure shows a normal grain size distribution. But, the presence of energy bias along some grain
boundaries results in abnormal growth of the microstructure. Comparing the grain boundaries around the tagged grain for mobility and energy bias cases, the visual analysis shows that the boundaries obtained with energy bias are more stretched and obtain irregular shapes. A larger curvature (convex outwards) of the grain boundaries is obtained for energy bias than a uniform smaller curvature for mobility bias condition. Therefore, with the additional curvature driven term, the microstructure evolution with energy bias is observed to be more violent than with mobility bias.

Fig. 4.11. Abnormal growth in the presence of GB energy bias of $\gamma_b/\gamma = 0.4$ around a grain located close to the center of the simulation cell. Four snapshots are shown when (a) 10000, (b) 5212, (c) 2161 and (d) 1312 grains are present
Quantitative analysis of the abnormal nature of growth for $\gamma_b/\gamma = 0.4$ is done with the help of the growth law, and the results are compared with the known case of normal grain growth. Fig. 4.12 represents that both the growth plots follow each other for certain period of time initially, after which the energy bias plot shows an upward rise, similar to the growth plot obtained for the mobility bias condition. The grain growth exponent for the energy bias case is observed to be about 1.12, similar to the case of mobility bias. This exponent is higher than the normal grain growth exponent ($n = 1.0$), resulting in abnormal grain growth. Thus, the simulation results show that the preexistence of energy bias in certain boundaries with uniform grain size distribution will promote abnormal grain growth.

Fig. 4.12. Time variation of average grain area with grain boundary energy bias.
The results obtained so far are performed with only one biased grain in the total microstructure. The individual effects of the influencing parameters are established properly. Now, further effort is made to simulate a more realistic system containing many biased grains. As initial geometrical bias does not enhance abnormal grain growth, the effect of grain boundary properties has been studied. Due to the violent nature of growth, the stability of the integrator for growth study with many grain boundary energy bias sites is doubtful. Therefore, the results obtained for mobility bias at many grain boundaries in the system is reported. This study is performed to capture the normal-abnormal-normal nature of growth as predicted for abnormal grain growth.

4.1.4 Effect of Mobility Bias in Presence of Several Biased Grains

Earlier result on mobility bias of a single grain indicates that the biased grain grows at the expense of the other grains in the microstructure. Now, the question arises: “Will the same nature of growth continue in the presence of many similar biased grains”? It is predicted that in the presence of many biased grains, the growth should go from an initial normal grain size distribution to an abnormal growth mode and then back to the normal growth mode (Fig. 3.4). This can be explained as follows. During the growth process when the biased grains are away from each other, these try to grow at the expense of the rest of the unbiased grains in the microstructure. As growth continues the growing biased grains come in contact with each other. This interaction of the growing boundaries of the biased grains will retard the growth process. The influence of these interactions collectively will result in a shift towards normal grain growth. Experimental result for annealing of nanocrystalline nickel has been reported to show this abnormal-normal growth phenomenon [75].
In order to simulate this typical nature of growth, a mobility bias \((M_b/M)\) of 7.0 is considered, where \(M_b\) is the mobility of the GBs surrounding the biased grains and \(M\) is the mobility of all the other GBs. A mobility bias value of 7.0 is considered, as this will definitely cause an abnormal growth for the biased grains. The study is conducted for different number of biased grains (e.g. 99, 250, 500, and 1000) in the system with initial uniform grain size distribution. Qualitative and quantitative discussions of the results are presented for each case. Qualitative analysis is done with visual inspection while there are approximately 10000, 5000, 2000, 1000, 600 and 150 grains left in the system. Quantitative discussion is based on the radius ratio evolution and growth law.

### 4.1.4.1 System with 99 Initial Biased Grains

Fig. 4.13 shows the snapshots of the microstructure evolution in the presence of 99 initial biased grains. It can be observed that initially the biased grains are more scattered and grow independently (Fig. 4.13. b).

![Fig. 4.13. Growth process in presence of 99 initial mobility biased grain with \(M_b/M=7\). Six snapshots are shown when (a) 10000, (b) 5168, (c) 2019 and (d) 1167, (e) 633 and (f) 181 grains are present. (Fig. Contd.)](image)
The average grain size of the scattered biased grains is observed to be close to the grain size of the single biased grain (Fig. 4.8. b) while approximately 5000 grains are left in the system. As the growth continues, the biased grains start influencing each other (Fig. 4.13. c-e), thereby reducing the growth rate. The final microstructure can be said to represent almost normal grain size distribution of the biased grains, while a few small grains are still left in the system.

Fig. 4.14. Time evolution of $\frac{R_b}{\langle R \rangle}$ with mobility bias of 7.0 for 99 initial biased grains.
The plot between $R_b/<Ra>$ and simulation time (Fig. 4.14) shows an interesting nature supporting abnormal to normal transition, where $<Ra>$ indicates the average grain size of the total grains in the microstructure. Initially, the radius ratio increases with a positive slope, showing that abnormal growth dominates. This is the region where most of the grains with biased grain boundaries are scattered in the matrix with minimum influence on each other. As time progresses the biased grains grow further and the high mobility boundaries influence each other. This process reduces the relative growth and the radius ratio decreases with time indicating a negative slope. In this region the normal growth mode is favored. Thus, there is a transition where the growth changes from abnormal to normal. Simulation results indicate that the transition occurs while there are approximately 2450 grains left in the system.

![Graph showing time variation of average grain area](image)

**Fig. 4.15.** Time variation of average grain area with 99 initial mobility biased grains.
The effect of more number of biased grains on the grain growth exponent is also studied. Fig. 4.15 shows the comparison between normal grain growth and growth with many mobility biased grains. The growth exponent is clearly observed to be much higher (~3.1) than the exponent for normal grain growth. The result obtained from Fig. 4.15 suggests that abnormal grain growth is favored with many grain boundary mobility biased grains with uniform grain size distribution. The analysis does not capture any abnormal-normal transition as monitored in the qualitative analysis and with radius ratio observation. Thus, further study is conducted with even higher number of biased grains.

### 4.1.4.2 System with 250 Initial Biased Grains

Fig. 4.16 shows the snapshots of the microstructure evolution with 250 initial biased grains. Similar observations are obtained for the qualitative analysis as reported for 99 initial biased grains. The average grain size of the biased grains is observed to be smaller than the previous condition for each corresponding grains left in the microstructure. The final microstructure (Fig. 4.16. f) can be said to represent almost normal grain size distribution containing mostly the biased grains. This visual observation certainly indicates the abnormal-normal growth mode.

The radius ratio variation (Fig. 4.17) also shows similar results as observed for the earlier case. Both normal and abnormal regions are properly defined in the curve. The final region of the plot indicates a radius ratio value of 1.0. This means that the average final grain size of the biased grains is equal to the average final grain size of the total grains in the microstructure. Therefore, the microstructure (Fig. 4.16. f) represents grains with biased grain boundaries only. All of them interact with each other with same mobility value for the boundaries (M_b/M = 7.0).
Fig. 4.16. Growth process in presence of 250 initial mobility biased grain with $M_b/M=7$. Six snapshots are shown when (a) 10000, (b) 4890, (c) 1949 and (d) 1109, (e) 691 and (f) 125 grains are present.

Fig. 4.17. Time evolution of $R_b/<R>$ with mobility bias of 7.0 for 250 initial biased grains.
Thus, this can be considered as a case of uniform mobility bias as $M_b/M = M_b/M_b = 1.0$. Each grain has the equal probability to grow. Also, uniform grain size distribution can be observed in this final microstructure. If grain growth is allowed to continue, normal grain growth can be expected to result. The transition point in the curve represents a microstructure with approximately 3250 grains left in the system.

![Graph](image)

**Fig. 4.18.** Time variation of average grain area with 250 initial mobility biased grains.

The grain growth exponent is studied by monitoring the time evolution of the average grain area during the growth process. It is interesting to note that the plot (Fig. 4.18) shows two different grain growth exponents. The comparison with normal grain growth indicates that the growth takes place abnormally with a higher growth exponent ($n \sim 3.3$). The value of $n$ is observed to be higher for 250 initial biased grains than for 99 initial biased grains condition. Later part of the plot toward the end shows a sudden
change in the value of $n$. This lowering of the growth exponent indicates that the nature of growth changes from abnormal to normal mode. Though the slope of the curve looks to be lower than the normal grain growth plot, it is difficult to report the representative quantitative value for the exponent. Further study is conducted with 500 and 1000 initial biased grains. The results are reported below.

4.1.4.3 System with 500 Initial Biased Grains

The visual observations (Fig. 4.19) for the growth of a system containing 500 initial mobility biased grain sites shows similar results as reported for 250 biased grains. The average grain size of the biased grains is observed to be smaller than for the previous initial mobility biased grain sites shows similar results as reported for 250 biased grains. The average grain size of the biased grains is observed to be smaller than for the previous
conditions for each corresponding grains left in the microstructure. The final microstructure (Fig. 4.19 f) can be said to represent a normal grain size distribution containing biased grains only.

The radius ratio study also captures the abnormal – normal growth mode as observed in the above microstructures (Fig 4.20). The final radius ratio value reaches 1.0 indicating that only biased grains are left at the end of the simulation. If the simulation is carried out further, normal grain growth will follow according to the earlier explanation. The maximum value of \(<R_b>/<R_a>\) is smaller than in the earlier cases. This suggests that as the number of grains with abnormal boundary mobilities increases in the system, they influence each other much sooner in the simulation than in the previous cases studied. The transition from abnormal to normal grain growth corresponds to a state where approximately 4500 grains are left in the system.

![Time evolution of \(R_b/<R>\) with mobility bias of 7.0 for 500 initial biased grains.](image)

**Fig. 4.20.** Time evolution of \(R_b/<R>\) with mobility bias of 7.0 for 500 initial biased grains.
Further study of the growth law indicates that both the stages of growth are clearly identifiable (Fig. 4.21). The initial stage of growth shows a higher value of growth exponent \( n \sim 3.4 \). In this region the plot represents abnormal growth. The latter stage showing normal grain growth is properly defined with a slope of \( \sim 0.3 \), lower than that for the growth of normal grains. The nature of this part of the curve shows a faster decrease in the exponent value, with the final part of the curve tending to become parallel to the normal grain growth plot.

**Fig. 4.21.** Time variation of average grain area with 500 initial mobility biased grains.

### 4.1.4.4 System with 1000 Initial Biased Grains

The snapshots for this system indicate a better representation of the abnormal – normal growth transformation (Fig. 4.22). The matrix is observed to be consisting of many growing grains distributed throughout the system. As the number of biased grains
is 10% of the total grains in the system, the interaction of the biased grains is observed much earlier during the simulation. The system with approximately 500 grains represents a grain structure with nearly uniform grain size distribution.

![Fig. 4.22. Growth mode in presence of 1000 initial mobility biased grain with $M_b/M=7$. Six snapshots are shown when (a) 10000, (b) 4952, (c) 2055 and (d) 1024, (e) 466 and (f) 157 grains are present.](image)

The radius ratio results indicate the abnormal – normal growth transition with a smaller increase in the maximum value of the average relative grain size of the biased grains (Fig. 4.23) This is due to the fact that a large number of biased grains interact with each other much earlier in the simulation. The abnormal to normal transition observed refers to a microstructure containing approximately 5050 grains in the microstructure.
This number of grains observed during the transition period is the highest in comparison with the earlier systems studied. Grains with uniform grain boundary properties in the microstructure are taken over by the biased grains. Therefore, the radius ratio plot reaches a value of 1.0 sooner, indicating only biased grains are left in the system. The growth with this microstructure shows normal grain growth as observed in Fig. 4.22. (f).

![Graph showing the time evolution of $\frac{R_b}{R_a}$ with mobility bias of 7.0 for 1000 initial biased grains.]

**Fig. 4.23. Time evolution of $R_b/R_a$ with mobility bias of 7.0 for 1000 initial biased grains.**

The average grain area plot during the growth process is shown in Fig. 4.24. Both abnormal and normal regimes are well defined in the plot. The growth exponent is observed to be greater than 1.0 (~2.7) in the initial part of the simulation, indicating abnormal grain growth is favored. The analysis of the later part of the plot indicates that growth due to the interaction of the abnormal grains changes to one with ~0.5, before tending to follow the growth plot for normal grains and the exponent can be said to be eventually approaching the value of 1.0 for normal grain growth. This explanation is
based on the growth plot tending to become parallel to the normal grain growth plot toward the end of the simulation.

![Graph showing time variation of average grain area with 1000 initial mobility biased grains.](image)

**Fig. 4.24.** Time variation of average grain area with 1000 initial mobility biased grains.

The normal distribution plot (Fig. 4.25) indicates an initial symmetric grain size distribution (10000). This symmetry is due to the initial Voronoi construction. As time proceeds the grain size distribution follows a more natural log normal grain size distribution. The peak of the individual plots decreases and the width broadens. The grain size distributions for many conditions are reported when the microstructure contains approximately 8000, 6000, 3000, 1000 and 200 grains left in the system. The peak and the area representing maximum number of grains in the microstructure shifts gradually towards the left of the initial normal distribution plot. However, the shift is observed to change its nature and move towards the right side for 200 grains left in the system.
Fig. 4.25. The grain size distribution plot in the presence of 1000 initial biased grains.
This right side shift from the previous nature of the plots is argued to be due to the influence of abnormal grains in the microstructure resulting in normal grain growth. A multimodal distribution is observed for 3000, 1000 and 200 plots.

![Radius ratio plot with respect to % Nb/Nt](image)

**Fig. 4.26. Radius ratio plot with respect to % Nb/Nt**

Further analysis is done to establish a relationship to predict the abnormal to normal transition due to the presence of biased grains in the initial microstructure. With the results obtained for the case of M_b/M = 7.0, the radius ratio (<R_b>/<R_a>) curves are plotted with the percentage of the ratio of the number of biased grains left in the system to the total number of grains left (N_b/N_t) at any particular time of the simulation. The plot (Fig. 4.26) indicates that the transition point changes for all the cases studied. The transition point is observed at a lower N_b/N_t ratio for lower number of biased grains in the initial microstructure, and vice versa. The radius ratio value decreases with increase in
the number of biased grains in the initial microstructure. This supports the fact that abnormal grains interact with each other much sooner in the presence of larger number of biased grains. This plot resembles the nature of the time evolution of the radius ratio plots discussed earlier.

From Fig. 4.26 no common characteristic can be predicted which will guide the abnormal – normal grain growth. Therefore, further analysis is done for the above condition. The variation of the radius ratio ($<R_b>/<R_a>$) with respect to the relative percentage of the area of the biased grains to the total number of grains in the microstructure ($A_b/A_t$) shows very interesting phenomena.

![Radius ratio plot with respect to % Ab/At](image.png)

**Fig. 4.27. Radius ratio plot with respect to % A_b/A_t**

The plots show (Fig 4.27) a slower increase in the radius ratio value with increase in the number of biased grains and the area ratio for all the cases studied, indicating that
abnormal grain growth occurs. The other half of the plot shows a gradual decrease in the radius ratio value, representing normal grain growth regime. But, the transition from abnormal – normal growth can be observed to be around a fixed ratio of the area of the biased grains to the area of the total grains, changing from about 40 to 50% as the number of biased grains is increased.

Table 4.1 summarizes the values for each case considered. It is interesting to note that the abnormal – normal transition is observed to occur when the area of the biased grains reaches around 50% of the total area of the microstructure.

Table 4.1. Simulation results for area ratio value showing abnormal – normal transition.

<table>
<thead>
<tr>
<th>Number of grains with initial mobility biased boundaries</th>
<th>% $A_b/A_t$ showing abnormal – normal transition</th>
<th>Approximate number of grains left in the system</th>
</tr>
</thead>
<tbody>
<tr>
<td>99</td>
<td>48.77</td>
<td>2450</td>
</tr>
<tr>
<td>250</td>
<td>49.76</td>
<td>3250</td>
</tr>
<tr>
<td>500</td>
<td>44.51</td>
<td>4500</td>
</tr>
<tr>
<td>1000</td>
<td>46.68</td>
<td>5050</td>
</tr>
</tbody>
</table>

Visual inspection is necessary (as area is involved) to comment on the probable phenomena for growth mode transformation. Figs. 4.28, 4.29, 4.30 and 4.31 show the snapshots of six different microstructures in and around the transition with 99, 250, 500 and 1000 initial biased grains respectively. Fig (c) for all the cases shows the microstructure close to transition. Careful investigation of the microstructures is very necessary to comment on the results observed from the simulation. Following are the microstructures observed for all the cases studied.
(A) 99 Initial Biased Grains:

Fig. 4.28. Microstructure evolution in and around the transition point in the presence of 99 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 4978, (b) 3512, (c) 2266, (d) 1726, (e) 1167 and (f) 633 grains are present.

(B) 250 Initial Biased Grains:

Fig. 4.29. Microstructure evolution in and around the transition point in the presence of 250 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 7747, (b) 5439, (c) 3437, (d) 1949, (e) 1109 and (f) 691 grains are present. (Fig. Contd.)
(C) 500 Initial Biased Grains:

Fig. 4.30. Microstructure evolution in and around the transition point in the presence of 500 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 7558, (b) 6436, (c) 4589, (d) 2930, (e) 1554 and (f) 1039 grains are present.

NOTE: * representative microstructure close to the abnormal to normal transition point.
(D) 1000 Initial Biased Grains:

Fig. 4.31. Microstructure evolution in and around the transition point in the presence of 1000 initial biased grains with $M_b/M=7.0$. Six snapshots are shown when (a) 7992, (b) 5390, (c) 4952, (d) 4032, (e) 3525 and (f) 2559 grains are present.

The microstructure evolution observations clearly indicate the formation of a well-defined percolating cluster of the grains with mobility bias values. Thus, more number of grain boundaries with mobility bias interacts with each other. The microstructures prior to the transition point (Fig. (a) and (b) for all cases) shows scattered mobility biased grains or a few clusters forming in the microstructure showing insignificant effect of the in-cluster interaction to the overall effect of the growth phenomena. The microstructures after the transition show a larger amount of interaction of the biased grain boundaries.
This effect reduces the overall growth rate of the biased grains and enhancing normal grain growth.
5. CONCLUSIONS

The following conclusions can be reported from the present study:

1. The presence of geometrical inhomogeneity does not promote abnormal grain growth.

2. Grain boundary properties (mobility and energy) have influential effect on the nature of growth. For both the conditions a threshold value is observed, which is the guiding factor for the nature of growth.

3. The threshold value is observed to be 2.3 for a microstructure containing grain boundary mobility bias with uniform grain size distribution. Abnormal grain growth is favored for mobility bias values above the threshold.

4. A similar result for grain boundary energy bias is observed. The threshold is observed to be approximately 0.8. Abnormal grain growth is favored for energy bias values below the threshold.

5. The influence of many mobility biased grains in the microstructure results in an abnormal – normal growth transition. This transition is observed to occur when the total area of all the biased grains accounts approximately 50% of the total area of the microstructure.

6. The abnormal – normal transition occurs when a well defined percolating cluster of the biased grains is observed in the microstructure. The interaction of the biased boundaries at this configuration shows a definite effect on the nature of growth. The mode changes from abnormal to normal.
REFERENCES


15. J.E. Burke and D. Turnbull, Progress in Metal Physics, 3 (1952) 220


35. A.D. Rollet and D. Raabe, Computational Materials Science, 21 (2001) 69


44. Y. Hayakawa and J.A. Szpunar, Acta Materialia, 45 (1997) 4713


47. F.J. Humphreys, Scripta Metallurgica et Materialia, 27 (1992) 1557


55. B. Radhakrishnan and T. Zacharia, Modelling and Simulation in Materials Science and Engineering, 10 (2002) 227


64. G. Gottstein and L.S. Shvindlerman, Scripta Metallurgica, 27 (1992) 1521
70. D. Weaire and J. Kermode, Philosophical Magazine B, 48 (1983) 245
Rakesh Kumar Behera was born in Cuttack, Orissa, India, on 3rd June 1978. He got his primary education at his home town Cuttack. After finishing his high school studies, he took one of the most rigorous competitive entrance examinations for engineering known as Orissa Joint Entrance Examination (OJEE). After qualifying in this examination he got admission to the Department of Metallurgical Engineering, Regional Engineering College (currently known as National Institute of Technology), Durgapur. He received his Bachelor of Engineering degree in Metallurgical Engineering from this Regional Engineering College in 2000. He came to the United States for his higher studies in August, 2002, and joined the graduate program in Mechanical Engineering at Louisiana State University (LSU), Baton Rouge, Louisiana, in Fall 2002. He is a candidate for the degree of Master of Science in Mechanical Engineering to be awarded during the commencement of August, 2004. After completing his master’s degree he plans to pursue his doctoral degree at the University of Florida, Gainesville.