A molecular dynamics study of grain boundary structures and their impacts on dislocation nucleation mechanisms

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A MOLECULAR DYNAMICS STUDY OF GRAIN BOUNDARY STRUCTURES AND THEIR IMPACTS ON DISLOCATION NUCLEATION MECHANISMS

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Table of contents

ABSTRACT .......................................................................................................................... I

ACKNOWLEDGEMENT ................................................................................................. III

CERTIFICATION ........................................................................................................ IV

LIST OF PUBLICATIONS ........................................................................................ V

LIST OF TABLES .......................................................................................................... VI

LIST OF FIGURES ....................................................................................................... VIII

CHAPTER 1 Introduction ............................................................................................... 1

1.1 Research background .............................................................................................. 1

1.1.1 Grain boundary .................................................................................................. 1

1.1.2 Dislocation-based deformation mechanism .................................................... 3

1.1.3 Molecular statics and molecular dynamics simulations ................................... 4

1.2 Research objectives ................................................................................................. 6

1.3 Structures of this thesis ........................................................................................... 6

Chapter 2 Literature review ......................................................................................... 8

2.1 Introduction ............................................................................................................. 8

2.2 GB structures and energies ................................................................................... 9

2.3 Grain boundary sliding ........................................................................................ 16

2.4 Dislocation nucleation from GBs ........................................................................... 20
2.5 Shear-coupled grain boundary migration .................................................. 25
2.6 Summary ..................................................................................................... 29

**Chapter 3 Research methodology** ................................................................. 30

3.1 Introduction .................................................................................................. 30
3.2 Molecular Dynamics simulations ................................................................. 30
3.3 Molecular statics ........................................................................................ 32
3.4 Potential energy .......................................................................................... 34
3.5 MC and MD simulation code LAMMPS ..................................................... 35
3.6 Visualisation tool ....................................................................................... 35
3.7 Common neighbour analysis ..................................................................... 36
3.8 Dislocation extraction algorithm ................................................................. 36
3.9 Summary ..................................................................................................... 37

**Chapter 4 Grain boundary structure and grain boundary energy** ............... 38

4.1 Introduction .................................................................................................. 38
4.2 Simulation model ........................................................................................ 39
4.3 Structures and energies of symmetric tile GBs .......................................... 42
    4.3.1 Structures and energies of STGBs with the tilt axis of [0 0 1] ............ 42
    4.3.2 Structures and energies of STGB with the tilt axis of [1 1 0] .......... 48
    4.3.3 Structures and energies of STGBs with the tilt axis of [1 1 1] ........ 55
4.3.4 Structures and energies of GBs with the <0 n l> tilt axis..............58
4.3.5 Structures and energies of STGBs with the <m m l> tilt axis.........59
4.4 Structures and energies of ATGBs..............................................61
   4.4.1 The analysis of ATGBs tilt with axes <1 2 l>........................62
   4.4.2 The analysis of ATGBs tilt with axes <1 3 l>.........................64
   4.4.3 The analysis of ATGBs tilt with axes <1 n l>.........................66
   4.4.4 The analysis of ATGBs tilt with axes <2 n l>.........................68
   4.4.5 The analysis of ATGBs tilt with other axes..........................70
4.5 Summary....................................................................................71

Chapter 5 Mechanism of dislocation nucleation from grain boundary........73

5.1 Introduction..................................................................................73
5.2 Simulation model.........................................................................74
5.3 Tensile deformation response of bicrystal models tilt with [0 0 1]......76
   5.3.1 The analysis of stress-strain of the GBs with the [0 0 1] tilt axis....76
   5.3.2 Mechanisms of dislocation nucleation from GBs with the [0 0 1]
       tilt axis......................................................................................77
5.4 Tensile deformation response of bicrystal models tilt with [1 \(\bar{1} 0]\)........85
   5.4.1 The analysis of stress-strain of the GBs with [1 \(\bar{1} 0]\) tilt axis........85
   5.4.2 Mechanisms of dislocation nucleation from GBs with the [1 \(\bar{1} 0]\) tilt
       axis.......................................................................................87
Chapter 6 Conclusions and Recommendations ........................................ 101

6.1 Analysis of GB structures and local minimal GB energies............... 101

6.2 Deformation mechanisms of GBs in Cu bicrystal GBs.................. 102

6.3 Recommendations for Future Work............................................ 104

References............................................................................................ 105

Affiliations............................................................................................ 108
Abstract

It is well known that grain boundaries play a significant role in determining the mechanical properties of polycrystalline materials. The study of the relationships between grain boundary (GB) structure and its associated deformation mechanisms is therefore of importance. This thesis investigates GB structures and GB energies over a wide range of GB misorientation angles and it investigates their influences on deformation mechanisms.

In the first part of this thesis, 1184 molecular statics (MS) simulations were conducted to study the structures and energies of the GBs of Cu and Al, taking into account their 66 tilt axes and various misorientation angles. The effects of GB tilt axis and misorientation angle on GB structure and GB energy were systematically investigated.

In the second part of this thesis, molecular dynamics (MD) simulations were performed to study the deformation mechanisms of symmetric tilt GBs with tilt axes of [0 0 1] and [1 1 0] in Cu under both ‘free’ and ‘constrained’ boundary conditions. The results indicate that stress states can have a profound effect on dislocation mechanisms. Dislocation nucleation was found to be independent of intrinsic GB structures. An automatic analysis of MD simulations provided detailed information on the dislocation nucleation and emission of GBs.

The results in this thesis contribute to our understanding of GB structure, GB energy and the dislocation nucleation mechanism. The GB energy data obtained in this thesis will be included in a crystal plasticity finite element model to
improve predictions of texture evolution and grain refinement during plastic deformation.
Acknowledgements

I would like to express my deep appreciation to my supervisors, Prof. Cheng Lu and Prof. Kiet Tieu, for their guidance and advice during my master’s study over the past two years. They have allowed me the freedom to direct this research project according to my own observations. This enabled me to develop the ability to think creatively and independently. I have always been motivated by their attitude toward my research and pleased by their advice. I feel truly honoured to have had them as my master’s supervisors.

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Thanks also to my parents and my family members for their strong support during my studies. I am grateful for their patience and understanding during my two years of study in Australia.
Certification

I, Nan Jiang, declare that this thesis submitted in fulfilment of the requirements for the conferral of the Master of Philosophy, from the University of Wollongong, is wholly my own work unless otherwise referenced or acknowledged. This document has not been submitted for qualifications at any other academic institution.

_____ (Signature)

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List of publications

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List of tables

Chapter 2

Table 2.1 List of the GB energies and the GBS threshold stresses of six GBs........ 19

Chapter 4

Table 4.1 Miller indices of the tilt axes used in the simulations.................... 41
Table 4.2. Simulated GB energies for STGBs with the same tilt axis of [0 0 1] and different misorientation angles $\theta$................................................................. 42
Table 4.3. Simulated GB energies for STGBs with the same tilt axis of [1 1 0] and different misorientation angles $\theta$................................................................. 48
Table 4.4. Simulated GB energies for STGBs with the same tilt axis of [1 1 1] and different misorientation angles................................................................. 56
Table 4.5 Tilt axes of $<0 \ n \ l>$................................................................. 58
Table 4.6 the tilt axes of $<m \ m \ l>$................................................................. 58
Table 4.7 Tilt axes of $<m \ n \ l>$................................................................. 61
Table 4.8 GB energies of Cu and Al for the [1 2 3] tilt axes and various misorientation angles................................................................. 62
Table 4.9 the GB energy as a function of rotation axes and misorientation angles ............................................................................................................. 64
Table 4.10 the GB energy as a function of rotation axes and misorientation angles ............................................................................................................. 66
Table 4.11 GB energy as a function of rotation axes and misorientation angles... .68

Table 4.12 GB energy as a function of rotation axes and misorientation angles
...........................................................................................................................................69

Chapter 5

Table 5.1 Schmid factor of resolved shear stress on the \{1 1 1\} \langle1 1 2\> slip system for the [0 0 1] tilt GBs.............................................................................................................................. .76
List of figures

Chapter 1

Fig. 1.1 The H-P relation and inverse H-P relation in terms of grain size and norminal strength ................................................................. 1

Fig. 1.2 Schematics of different dislocations: (a) Shockley partial dislocation [9], (b) Frank partial dislocation, (c) extended dislocation and (d) Lomer-Collrel dislocation ........................................................................................................ 4

Chapter 2

Fig. 2.1 Symmetric GB structures tilted with [0 0 1] in Cu at 0 K .................. 9

Fig. 2.2 Nineteen equilibrium symmetrical boundary structures tilted with <1 1 0> .................................................................................................................... 12

Fig. 2.3 Four Σ5 ATGB structures in Cu .................................................................................. 13

Fig. 2.4 Two Σ11 ATGB structures in Al ........................................................................ 13

Fig. 2.5. The calculated GB energy of Ni as a function of misorientation angle around (a) <001> tilt axis. (b) <110> tilt axis ................................................................. 14

Fig. 2.6 GB energy as a function of inclination angle in Cu and Al, and the fits for the values by Eqn. (2-1) ........................................................................................................... 15

Fig. 2.7 GB energy of (a) Σ5 and (b) Σ13 ATGBs with the <100> tilt axis as a function of φ .................................................................................................................. 16

Fig. 2.8 GB energy of (a) Σ9 and (b) Σ11 ATGBs with the <110> tilt axis as a function of φ .................................................................................................................. 16
Fig. 2.9 The sliding behaviour under different conditions........................................18

Fig. 2.10 Snapshot of Al $\Sigma 3$ GB structures of (a) pure GB; (b) 2% vacancies GB; (c) 15% vacancies GB.......................................................... 19

Fig. 2.11 Full dislocation nucleation loops during uniaxial tension of Al.............. 20

Fig. 2.12 Uniaxial tensile deformation of the 53.1° GB in Cu model .................... 22

Fig. 2.13 Uniaxial tensile deformation of STGBs in Cu........................................ 24

Fig. 2.14 Dislocation nucleation from STGB and ATGB in Cu $\Sigma 5$..................... 24

Fig. 2.15 Calculated GB positions and shear stress at different temperatures for SC-1............................................................................................................... 26

Fig. 2.16 Calculated GB positions and shear stress at different temperatures for SC-2................................................................. 26

Fig. 2.17 Critical stress, SCM mode and whether tilt axis-oriented atomic shuffling exists for the SCM process of the [100] group STGBs at 0.1 K......................... 27

Fig. 2.18 Shear stress and GB displacements as a function of time of the $\Sigma 85$ and $\Sigma 13$ GBs.................................................................................................................. 28

Fig. 2.19 (a) Migrations and (b) GBS as functions of time at different temperatures for shearing along [1 3 0]......................................................................................... 29

Chapter 3

Fig. 3.1 Flow chart for conjugate gradient algorithm used in the energy minimization calculations................................................................. 33

Chapter 4
Fig. 4.1 Bicrystal symmetric tilt GB model................................................................. 40

Fig. 4.2 Stereographic triangle showing 66 crystallographic orientations of the tilt axes.......................................................................................................................... 41

Fig. 4.3 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [0 0 1] tilt axis.................................................................................................. 45

Fig. 4.4 GB energy as a function of the orientation angles $\theta$ for the Cu STGBs with the [0 0 1] tilt axis compared with the results reported by Mishin et al........ 45

Fig. 4.5 Sixteen STGB structures in Cu with the [0 0 1] tilt axis.................................... 47

Fig. 4.6 Eight GB structures in Al with the [0 0 1] tilted axis....................................... 47

Fig. 4.7 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [1 1 0] tilt axis................................................................................................. 51

Fig. 4.8 GB energy as a function of the orientation angles $\theta$ for the Cu STGBs with the [1 1 0] tilt axis compared with the results reported by Zhang...................... 51

Fig. 4.9 Fifteen GB structures in Cu with the tilt axis of [1 1 0].................................... 54

Fig. 4.10 Six GB structures in Al with the tilt axis of [1 1 0]........................................ 55

Fig. 4.11 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [1 1 1] tilt axis................................................................................................. 57

Fig. 4.12 Six GB structures in Cu with the tilt axis of [1 1 1]....................................... 57

Fig. 4.13 GB energies of Cu and Al as a function of the misorientation angle for the GBs for [0 1 2] and [0 2 3] tilt axes............................................................................. 59

Fig. 4.14 Four typical GB structures in Cu with the tilt axis of <0 n l>................. 58
Fig. 4.15 GB energies of Cu and Al as a function of the misorientation angle for the GBs for [1 1 3] and [5 5 1] tilt axes................................................................. 59

Fig. 4.16 Two GB structures in Cu and Al tilt with <m m l>.................................. 60

Fig. 4.17 Bicrystal model with asymmetric tilt GB............................................. 62

Fig. 4.18 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [1 2 3] and [1 2 4] tilt axes......................................................... 62

Fig. 4.19 Two GB structures in Cu and Al tilt with <1 n l>.................................... 64

Fig. 4.20 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [1 3 4] and [1 3 5] tilt axes......................................................... 64

Fig. 4.21 Snapshot of GBs in Cu and Al tilt with <1 3 l>..................................... 65

Fig. 4.22 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [1 5 6] and [1 10 11] tilt axes....................................................... 67

Fig. 4.23 Snapshot of GBs in Cu tilt with <1 n l>................................................. 67

Fig. 4.24 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [2 3 4], [2 6 7], [2 9 10] and [2 4 5] tilt axes................................. 68

Fig. 4.25 Snapshot of GBs in Cu and Al tilt with <2 n l>..................................... 69

Fig. 4.26 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [4 5 6] and [7 8 9] tilt axes.................................................... 71

Fig. 4.27 Snapshot of GBs in Al tilt with <m n l>.................................................... 71

Chapter 5
Fig. 5.1 Stress-strain curves of Cu bicrystal models with the <0 0 1> tilt axis and various misorientation angles under tension loading with free boundary condition along X and Z directions.................................................................78

Fig. 5.2 (a) Maximum tensile stress and (b) maximum resolved shear stress versus misorientation angle for Cu bicrystal models under tensile deformation with free boundary conditions along the X and Z directions........................................78

Fig. 5.3 Dislocation activities and atomistic configurations for $\Sigma 17$ (4 1 0) GB at 1 K during free tensile deformation process.................................................................80

Fig. 5.4 Dislocation activities and atomistic configurations for $\Sigma 17$ (5 3 0) GB at 1 K during tensile deformation process.................................................................82

Fig. 5.5 Stress-strain curves of Cu bicrystal models with the <0 0 1> tilt axis and various misorientation angles under tension loading under constrained boundary conditions along X and Z directions.................................................................83

Fig. 5.6 Dislocation activities and atomistic configurations for $\Sigma 5$ (2 1 0) GB at 1 K during tensile deformation.................................................................84

Fig. 5.7 (a) Maximum tensile stress and (b) maximum resolved shear stress versus the misorientation angle in Cu bicrystals under tensile deformation with constrained boundary condition.................................................................85

Fig. 5.8 Stress-strain curves of Cu bicrystal models with the <110> tilt axis and various misorientation angles under tension loading with free boundary conditions along X and Z directions.................................................................87
Fig. 5.9 (a) Maximum tensile stress and (b) maximum resolved shear stress versus the misorientation angle in Cu bicrystals with the $<110>$ tilt axis under tensile deformation with free boundary condition........................................................................86

Fig. 5.10. Dislocation activities and atomistic configurations for (a) $\Sigma 19$ (1 1 6) GB, (b) $\Sigma 33$ (2 2 5) GB and (c)-(d) $\Sigma 17$ (2 2 3) GB during tensile deformation with free boundary conditions..................................................................................................................88

Fig. 5.11 Dislocation activities and atomistic configurations for (a)-(b) $\Sigma 9$ (1 1 4) and (c)-(d) $\Sigma 11$ (1 1 3) GBs during tensile deformation; (e)-(f) a detailed inspection of the snapshots of the evolution of C SU.............................................................................................90

Fig. 5.12. Dislocation activities and atomistic configurations for (a) $\Sigma 3$ (1 1 1) GB and (b)-(c) $\Sigma 171$ (11 11 10) GBs during tensile deformation.................................................................92

Fig. 5.13. Dislocation activities and atomistic configurations for $\Sigma 11$ (3 3 2) GB at 1 K during tensile deformation process...........................................................................................................96

Fig. 5.14. Dislocation activities and atomistic configurations for (a) $\Sigma 9$ (2 2 1) GB, (b) $\Sigma 19$ (3 3 1) GB, (c) $\Sigma 73$ (6 6 1) GB during tensile deformation.................................96

Fig. 5.15. Dislocation activities and atomistic configurations for $\Sigma 9$ (2 2 1) GB during constrained tensile deformation.................................................................................................................97
CHAPTER 1

Introduction

1.1 Research background

1.1.1 Grain boundary

A grain boundary (GB) is a solid–solid interface in polycrystalline materials, and there is a close correlation between GB and a material’s physical, chemical and mechanical properties. GB plays a vital role in determining the properties of polycrystalline materials. Researchers have studied the relationships between GB structures and mechanical properties, including GB sliding, dislocation emission and annihilation, grain coalescence, GB migration and dislocation pile-ups at the GBs [1, 2].

According to previous research, grain size has a strong influence on mechanical strength. The relationship between grain size and nominal strength is depicted schematically in Fig. 1.1 [3, 4], which shows that grain size has a significant influence of the mechanism of metallic materials.

![Fig. 1.1. The H-P relation and inverse H-P relation in terms of grain size and nominal strength.[4]](image)
As shown in Region 1 in Fig. 1.1, the strengthening behaviour of conventional metallic materials with a grain size larger than 100 nm is well characterised by the widely referenced Hall-Petch (H-P) relationship. In this region, yield strength rises with decreasing grain size. This is because the density of the GB increases significantly with a decrease in average grain size, giving rise to increased strength. In Region 2, the homogeneous intragranular nucleation of dislocations is limited, and the H-P relation becomes weak. In Region 3, grain size is usually less than 10 nm, and the strength of the material decreases as grain size decreases. This phenomenon is called the inverse H-P relationship. It is believed that in Region 3 dislocation nucleation is restricted and GB-mediated processes, such as GB migration, GB sliding and grain rotation, are the primary deformation regimes.

The influence of GB on a material’s properties is mainly determined by the boundary structures and GB energy (excess energy per unit GB area). Several studies, including theoretical, computational and experimental studies, have examined the GB structures and energies of various materials. However, GBs with a wide range of tilt axes and misorientation angles still need more in-depth analysis.

In the past two decades, ultrafine-grained (UFG) materials and nanostructured materials have been developed. Usually, these materials have high strength, but unfortunately low ductility. Many engineering applications call for materials with both high strength and high ductility. How to produce such materials in large volumes is therefore a challenging research topic. An ARC Discovery project (DP170103092) “Large-volume gradient materials: manufacturing and deformation mechanism” is being conducted by our research group, aiming at developing an innovative low-cost and high productivity process in response to
this challenge. One aim of this project is to develop a crystal plasticity finite
element method (CPFEM) model to better understand the effects of texture and
grain size distribution on the deformation mechanisms of gradient materials. To
accomplish this aim, the GB energies for various tilt axes and misorientation
angles need to be calculated and included in the CPFEM model.
In this thesis, 1184 molecular statics (MS) simulations were conducted to study
the structures and energies of the GBs of Cu and Al with 66 tilt axes and various
misorientation angles. In addition, MD simulations were performed to study
dislocation nucleation from GBs.

1.1.2 Dislocation-based deformation mechanism

Defects exist in all real crystals, and the existence of defects influences the atomic
arrangements of bicrystal GBs. The properties of crystalline materials can be
greatly modified by the presence of defects. For example, point defects, including
interstitials, vacancies and their clusters, play a significant role in the initiation of
plastic deformations in crystalline metals [5-7]. Additionally, line defects called
dislocations are crucial defects in crystalline solids. There are two types of
dislocations, namely glides and climbs. Glides result in slips and are the most
common manifestations of plastic deformation in crystalline solids. Climbs are
movements of the dislocation perpendicular to the slip plane, and are important
forms of plastic deformation at high temperatures [8]. Four types of dislocation
are shown in Fig. 1.2. Shockley partial dislocation [9], as shown in Fig. 1.2 (a),
exists in FCC metallic materials and the displacement vector is \( \mathbf{b}=a/6<1 1 2> \). As
shown in Fig. 1.2 (b), Frank partial dislocation in FCC systems is defined as \( \mathbf{b}=a/3[1 1 1] \), which could only move on its glide cylinder. The extended dislocation shown
in Fig. 1.2 (c) is a combination of Shockley partial dislocations and stacking faults.
Lomer-Cottrell dislocations [10-12] are partial dislocations which are sessile and immobile on the slip plane.

Fig. 1.2 Schematics of four types of dislocation: (a) Shockley partial dislocation [9], (b) Frank partial dislocation, (c) extended dislocation and (d) Lomer-Collrel dislocation [12].

1.1.3 Molecular statics and molecular dynamics simulations

With the burgeoning development of computational capability, atomistic simulations have been conducted to examine the mechanical properties of nanostructured materials and progressively obtain a better understanding of deformation mechanisms at the atomic scale. Atomistic simulations, including molecular statics (MS) calculations and molecular dynamics (MD) simulations, are used to investigate the properties and behaviours of GBs.
MS calculation is a process of relaxing the configuration of atoms by applying the conjugate gradient method to minimise the total energy of the simulated domain. This will be further explained in Section 3.3.

MD simulation has become an effective way to simulate the behaviours of defects in crystals under conditions of applied deformation, loading or temperature change. With the remarkable developments in post-processing technology such as visualisation tools [13] and the sophisticated automated techniques of dislocation detection [9, 14, 15], MD simulations provide insights into the underlying deformation mechanisms at the atomic level which cannot be directly observed in experiments. Large numbers of MD simulations have indicated that this approach has achieved a high level of success. The following deformation mechanisms at the atomic level have been identified: dislocation nucleation and annihilation at the GB [16, 17]; prediction of mechanical twinning in Al [18]; crossovers from dislocation-dominated deformation to GB-based deformation [19]; shear bands [20] and the influence of interactions between ductile dimples and shear regions on fracture surfaces [21].

In this thesis, bicrystal GB models were developed for both MS calculations and MD simulations. MS calculations were first conducted to model appropriate GB structures with minimum GB energies for Cu and Al. MD simulations were then performed to analyse the deformation mechanisms of GB, including dislocation nucleation activities.
1.2 Research objectives

In this thesis, the overall aim is to deeply understand the relationships between the GB structures, GB energies and deformation mechanisms of FCC metallic materials. The specific aims of this thesis are:

(1) to calculate the GB energies of FCC metals (Cu and Al) at a wide range of tilt axes and misorientation angles. Based on the calculation results, a table will be built showing GB energy as a function of the tilt axes and misorientation angles and implemented in the CPFEM model.

(2) to identify the GB characteristics and structures of FCC metals (Cu and Al) at various tilt axes and misorientation angles

(3) to study the effects of GB structures and energies on the plastic deformation mechanisms of materials (dislocation nucleation) under uniaxial loading.

1.3 Structure of this thesis

This thesis has been organised as follows.

Chapter 2 critically reviews the previous understanding of GBs, including GB structures, GB energies and GB-mediated deformation mechanisms under uniaxial tension/shear conditions.

Chapter 3 gives a brief introduction to the research methodology used in this thesis, including the MD simulation methodology, the potentials used in molecular dynamic simulations and visualisation technologies.

Chapter 4 studies the GB structures and energies of 66 groups of symmetric GB models with various tilt axes and misorientation angles for Cu and Al.
Chapter 5 studies the dislocation nucleation mechanisms of GBs under uniaxial loading ‘free’ and ‘constrained’ boundary conditions. The dislocation nucleation mechanisms are discussed and classified based on different orientation ranges.

Chapter 6 concludes the work of this thesis and proposes future areas of research.
Chapter 2

Literature review

2.1 Introduction

During manufacturing processes, the atoms of crystalline materials gather together and form into groups in particular orientations called crystalline orientations. A group of atoms forms a region named a grain and the area between the different regions is the grain boundary (GB) [22]. The orientation of each grain changes across the GB. There are two types of tilt GBs: symmetric tilt GBs (STGBs) and asymmetric tilt GBs (ATGBs). In STGBs the orientations of the upper and lower grains are rotated around the tilt axis at equal misorientation angles ($\theta/2$), but one is rotated in a counterclockwise direction and the other in a clockwise direction. In other words, the orientations of the two grains are symmetrical with respect to the tilt axis. This will be described in Section 4.2. In ATGBs the orientation of the upper grain is tilted with an inclination angle $\phi$ relative to the orientation of the lower grain and this will be described in Section 4.5.

The coincident site lattice (CSL) [23, 24] notation is an important tool to characterise the GB structures because the patterns of CSL lead directly to the definable periodic structures at the GB. The density of coincident lattice points is defined as $\Sigma$. The CSL methodology has been applied to analyse the structures of GBs in this thesis.
2.2 GB structures and energies

It is well known that GBs profoundly affect the performance of nanocrystalline metals [25, 26]. To investigate mechanical deformation behaviour, it is essential to understand GB structures and to calculate the corresponding GB energies. Cahn et al. [27] simulated over 20 symmetrical tilt GBs in Cu with the misorientation angle $\theta$ values varying from 18.9° to 79.6° and $\Sigma$ values of between 5 and 101. They utilised the CSL method, classifying boundaries and every single CSL GB, can be defined by the indices $(h \ k \ 0)$ of the GB plane. All ground-state structures with the minimum GB energy were determined using MS calculations.

![Fig. 2.1 Symmetric GB structures tilted at [0 0 1] in Cu at 0 K. [27]](image)

As shown in Fig. 2.1, all the GBs were composed of topologically identical kite-shaped E structural units (SUs). The only differences between these GBs were the arrangements of the kite-shaped units’ separation distances and their positions relative to the GB planes. As shown in Fig. 2.1 (a), the $\Sigma 37 \ (6 \ 1 \ 0) \ \theta = 18.9^\circ$ GB is a relatively low-angle GB, and the dislocations were formed by the E SUs and their Burgers vectors were $\mathbf{b} = [1 \ 0 \ 0]$. Similarly, a relatively high-angle $\Sigma 41 \ (5 \ 4 \ 0) \ \theta = 77.3^\circ$ GB, as shown in Fig. 2.1 (d), has dislocations of $\mathbf{b} = - \frac{1}{2}[1 \ 1 \ 0]$. 
Rittner and Seidman [28] investigated twenty-one $<1\ 1\ 0>$ symmetric tilt GBs by using atomistic simulations to identify both the equilibrium and metastable structures at 0 K. The GB structures with tilt angles of between 0° and 109.47° (Fig. 2.2 (a)-(m)), contained four SUs: (1) A SU from $\Sigma1\ (0\ 0\ 1)\ \theta=0°$, which is called perfect crystal orientation; (2) A’ SU from $\Sigma43\ (3\ 3\ 5)\ \theta=80.63°$, which is identical to the A SU but rotated by 90°; (3) C SU from $\Sigma11\ (1\ 1\ 3)\ \theta=50.48°$; and (4) D SU from $\Sigma3\ (1\ 1\ 1)\ \theta=109.47°$. When the tilt angle is beyond 109.47°, the E and E’ SUs exist in the GB structures, as shown in Fig. 2.2 (n)-(u).
Several atomistic simulations have focused on symmetric GB structures, energies and other properties. However, reports on asymmetric GBs are relatively few. Tschopp and McDowell [29, 30] investigated the structures and energies of ATGBs in both Cu and Al, and they compared their energy relationships based on faceting into the two STGBs in each system. Fig. 2.3 shows four Σ5 asymmetric tilt GBs (ATGB) of Cu, and Fig. 2.4 provides details of two Σ11 ATGBs of Al. Obviously, each ATGB in Cu and Al can facet into two corresponding symmetric tilt GBs. For the Σ5 (100)$_1$/(430)$_2$ φ = 18.43° ATGB in Cu, as shown in Fig. 2.3 (b), the GB contains C and B’ SUs in equal proportions. For the Σ11 (2 2 5)$_1$/(4 4 1)$_2$ φ=54.74 ATGBs, as shown in Fig. 2.4 (a), dislocations are faceted into the SUs of Σ11 (1 1 3) GB and Σ11 (3 3 2) GBs. The Σ11 (5 5 7)$_1$/(7 7 1)$_2$ φ = 70.53° ATGB, as shown in Fig. 2.4 (b), comprised E and D SUs only.
Experiments and atomistic simulations have been conducted to prove that there is a correlation between GB structure and GB energy [30-34]. For example, Sangid et al. [33] simulated various twist and tilt GBs and the results are shown in Fig. 2.5.

In Fig. 2.5 (a), the calculated GB energies were symmetrical about the misorientation angle of $\theta=90^\circ$, and $\Sigma 5 \theta=36.87^\circ$ and $126.87^\circ$ have local minimum energies. Fig. 2.5 (b) shows the GB energies with respect to a group of tilt GBs, which were tilted along the $<110>$ axis. The lowest value exists in the $\Sigma 3 (1 \bar{1} 1)$ $\theta=109.5^\circ$ GB, which was mainly due to its very simple defect structures and is known as a coherent twin boundary (CTB).
Fig. 2.5. The calculated GB energy of Ni as a function of misorientation angle around (a) <001> tilt axis. (b) <110> tilt axis. [33]

For ATGBs, Tschopp et al. [29, 35] have tried to explain the relationship between structure and GB energy. Their assumption was that the energy of an asymmetric GB could be correlated to the two symmetric GBs’ energies, as described by Eqn. (2-1), which is also related to the inclination angle (ϕ). For example, through simulating twenty-five Σ3 ATGBs in the <1 1 0> system, it was concluded that the Σ3 ATGBs can facet into the CTB and symmetric incoherent twin boundary (SIGB). The GB energies calculated using Eqn. (2-1) were plotted against the GB energy obtained from their simulation results, as shown in Fig. 2.6. The fitted GB energy and calculated value of Cu do not match very well for ϕ>70.53°, as a result of the 9R phase dissociated from the GB region.

\[ \gamma_\phi = \gamma_{CTB} \cos \phi + \gamma_{SIGB} \sin \phi \]  

(2-1)
Tschopp et al. [29] further investigated ATGBs. ATGB energies were calculated as a function of the inclination angle $\phi$. The results were compared with the energy relationships of the two STGBs, based on the faceting in each system. They subsequently developed an equation to calculate the ATGBs’ energies.

$$
\gamma_{ATGB, \phi} = \gamma_{STGB, 1} \left[ \cos \phi - \sin \phi \left( \frac{\cos \alpha}{\sin \alpha} \right) \right] + \gamma_{STGB, 2} \left( \frac{\sin \phi}{\cos \alpha} \right) \tag{2-2}
$$

where $\gamma_{ATGB, \phi}$ is the ATGB energy, $\gamma_{STGB, 1}$ and $\gamma_{STGB, 2}$ are the STGB energies, and $\alpha$ is the inclination angle which separates two STGBs of the same CSL system (for the $<1 1 1>$ system, $\alpha=30^\circ$; for the $<1 0 0>$ system, $\alpha=45^\circ$, and for the $<1 1 0>$ system, $\alpha=90^\circ$).
Fig. 2.7 GB energy of (a) $\Sigma 5$ and (b) $\Sigma 13$ ATGBs with the $\langle 100 \rangle$ tilt axis as a function of $\phi$. [29]

Fig. 2.8 GB energy of (a) $\Sigma 9$ and (b) $\Sigma 11$ ATGBs with the $\langle 110 \rangle$ tilt axis as a function of $\phi$. [29]

Fig. 2.7 and Fig. 2.8 give the calculated GB energies of four CSL systems. The $\Sigma 5$ and $\Sigma 13$ GBs in the $\langle 100 \rangle$ system agreed with the energy relationship (Eqn. (2-1)) mentioned above, but the $\Sigma 9$ and $\Sigma 11$ GBs in the $\langle 110 \rangle$ systems deviated from the idealised relationship of energy, indicating that the dislocations faceting into the structures of the two symmetric counterparts were not energetically favourable.

### 2.3 Grain boundary sliding

Grain boundary sliding (GBS) implies that one grain translates over another grain rigidly to the boundary interface parallel. GBS is an important mechanism for
deformation for superplastic forming (SPF) [32] and quick plastic forming (QPF) [33] at elevated temperatures. For polycrystalline materials, when grain size decreases to the nanometre scale [34] and the temperature of deformation is relatively high [35, 36], GBS mediates the plastic flow.

Qi et al. [37] studied GBS over different shear forces and GB misorientation angles \( \theta \) in Al at 750 K. There were three phenomena observed, as shown in Fig. 2.9 (a). Under a low applied force, no sliding was observed, indicating that there was threshold stress-type behaviour. Under intermediate applied forces, the number of GBS increased linearly with time. Under high applied forces, the amount of GBS increased parabolically with time. However, the misorientation angle (\( \theta \)) did not correlate with the amount of sliding (Fig. 2.9 (b)). In their research, in all GB structures the velocity of sliding varied linearly with the applied stress (Fig. 2.9 (c) (d)). A linear fit of this relationship did not intersect the stress axis at the origin, indicating the existence of a critical threshold stress. The applied stress must be larger than the critical stress to initiate GBS.
Du et al. [38] conducted MD simulations at 750 K to investigate the influences of vacancies on GBS behaviour in the boundary vicinity of Al bicrystals (Fig. 2.10). The threshold stresses for the GB sliding of one STGB and five ATGBs were computed under various vacancy concentrations (Table 2.1). They found that the low-energy $\Sigma 3$ GB presented remarkably less sliding than the other, relatively high-energy GBs without vacancies. The threshold stress for GBS increased with a decrease in the addition of vacancies to $\Sigma 3$ GBs, which improved the diffusivity of the GB. This effect was enhanced by the rise of vacancy concentrations. It has been found that GB diffusivity and GB sliding are negligible for high energy GBs, due to atom mobility in these boundaries.
Fig. 2.10. Snapshot of Al $\Sigma 3$ GB structures of (a) pure GB; (b) 2% vacancies GB; (c) 15% vacancies GB. [38]

Table 2.1 List of the GB energies and the GBS threshold stresses of six GBs. [38]

<table>
<thead>
<tr>
<th>GB structure</th>
<th>GB energy at 300 K Pure GB (mJ/m²)</th>
<th>GBS threshold stress at 750 K (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pure GB</td>
<td>GB+2%V</td>
</tr>
<tr>
<td>$\Sigma 3$</td>
<td>0.07</td>
<td>1.18</td>
</tr>
<tr>
<td>110_90</td>
<td>0.43</td>
<td>0.88</td>
</tr>
<tr>
<td>110_10</td>
<td>0.45</td>
<td>0.69</td>
</tr>
<tr>
<td>110_35</td>
<td>0.51</td>
<td>0.02</td>
</tr>
<tr>
<td>110_55</td>
<td>0.52</td>
<td>0.07</td>
</tr>
<tr>
<td>110_25</td>
<td>0.55</td>
<td>0.02</td>
</tr>
</tbody>
</table>

It can be seen in Fig. 2.9 (a) that the GBS resistance of GB has a close relationship with the GB energy. Chandra et al. [39] proposed a direct relationship between GB energy and the distance of GBS in Al STGBs. Namely, the sliding distance decreases with decreasing GB energy, thus confirming the conclusion of Qi et al. [37]. This finding has been confirmed in a large number of studies on thermally-activated GBS, indicating that faster GB sliding occurs for GBs with a higher self-diffusion rates, which correlates to both GB volume and GB energy.

Sansoz and Molinari et al. [40, 41] studied the influence of GB structures on the GB sliding mechanism. They used the quasicontinuum (QC) method [42, 43] and their simulation results showed that: (1) If there was no thermally activated mechanism involved, GB energy could not be viewed as the relevant parameter to predict sliding on high-angle boundaries at the nanometre level; and (2) The E SUs
can serve as a source of onset of sliding through atomic shuffling in the period of the tilt GBs.

2.4 Dislocation nucleation from GBs

GBs can serve as a source of dislocation nucleation. This has been well established both by atomistic simulations and via experimental observations. Spearot et al. [44] applied MD simulation to study the influence of tensile stress on <0 0 1> STGBs in the Al $\Sigma 5$ (3 1 0) $\theta=36.9^\circ$ GB. It is worth noting that the nucleation of full dislocation loops from boundaries can be observed because of their relatively low interfacial energy. Fig. 2.11 show the full dislocation nucleated from the GB during the process of tensile deformation. Fig. 2.11 (f) shows two distinct points during the nucleation process: an extended dislocation from the upper lattice region and a full dislocation loop from the lower lattice region.

![Fig. 2.11 Full dislocation nucleation loops during uniaxial tension of Al. [44]](image)

Spearot et al. [45] also used bicrystal models with STGB structures to study the deformation behaviour of the interface plane under a uniaxial tensile at 10 K and
300 K. The A-D, circled in Fig. 2.12, represents the specific points of the interest. Fig. 2.13 (a) shows that the bicrystal interface structure evolved prior to the dislocation nucleation events. Specifically, the length of the intrinsic stacking fault (ISF) facets became shorter as the tensile stress increased. In Fig. 2.12 (b), additional tensile strain caused partial edge dislocations which nucleated from the intersection of the ISF facets and the interface, and partial edge dislocation nucleation was connected back to the interface through an extrinsic stacking fault (ESF). With increasing tensile strain, the nucleation of partial edge dislocations faceted into the lattice region from the ISF oppositely, as shown in Figs. 2.13 (c) and (d). Further tensile strain caused trailing partial dislocation nucleation, which started from both sides of the GB plane, resulting in a transformation from ESF to ISF. Meanwhile, ISF facets were completely absorbed by the boundary. It could be concluded that the presence of ISF facets facilitated partial dislocation nucleation from the secondary slip plane.
Tschopp and McDowell [46] used atomistic simulations to investigate dislocation nucleation from the Σ3 ATGBs under uniaxial tension at 10 K. Their work revealed that the mechanisms of dislocation nucleation clearly changed in response to changes to the inclination angle for identical misorientations. As shown in Fig. 2.13, for φ≤35.26° (relatively low inclination angles) the process of dislocation
nucleation occurred from different slip planes compared with the planar dissociations, and the stress associated with nucleation events was relatively high. For $35.26^\circ < \phi < 70.53^\circ$ (intermediate inclination angles), the processes of dislocation nucleation and emission started from the same slip plane where the partial dislocations dissociated and the required stress for the dislocation nucleation was low. For $\phi \geq 70.53^\circ$ (high inclination angles) the extended dissociations of the boundary resulted in an increase of volume in the 9R phase. In their simulation results, the dislocation nucleation only occurred in one of the adjoining crystals for the $\Sigma 3$ ATGBs.

\begin{align*}
\Phi &= 10.02^\circ \\
\Phi &= 54.74^\circ
\end{align*}

(i)

(ii)
Zhang et al. [47] conducted MD simulations to study both symmetric and asymmetric Σ5 GBs in Cu. Fig. 2.14 (a) shows that, for the STGBs, dislocations emitted into both upper and lower grains as the maximum tensile stress was reached. On the other hand, for the ATGBs (Fig. 2.14 (b)), the partial dislocations preferentially nucleated into the lower grain lattice as the imposed tensile stress increased to its maximum. This phenomenon can be explained by the fact that the different orientation angles of upper and lower grains resulted in different Schmid factors. To accommodate further tensile strain, the slip system in the upper grain was also activated.
2.5 Shear-coupled grain boundary migration

Li and Edwards initially observed the shear-coupled grain boundary migration (SCM) in low-angle GBs in 1950 [48]. Since then, the shear-induced motion of high-angle GBs has also been found in Al [49] and Zn [50]. The basic concept of coupled migration is that the shear stress applied on a GB plane causes a GB’s normal motion. Cahn et al. [51] proposed a geometric model to elucidate this coupling effect. In their model, the coupling factor $\beta$ is given by the ratio of relative grain translation $S$ to the GB normal motion $H$. That is, $\beta = S / H$. In subsequent research, extensive experimental observations and atomistic simulations provided significant insights into the elementary mechanisms of shear-coupled GB motion. For example, using MD simulations Cheng et al. [52] investigated the effects of the structural multiplicity of the symmetric tilt $\Sigma 5 (3 1 0)$ GB on its coupled motion behaviour at temperatures ranging from 300 K to 600 K. According to their simulations, three types of GB behaviours were present. The first one was associated with a typical stop-and-go GB motion and stick-slip stress behaviour, as shown in Fig. 2.15. The second GB behaviour corresponded to the second starting configuration (SC-2) cases at 300 K and 400 K, as well as the first part (slope=-0.74 in Fig. 2.16 (c)) of that at 500 K (Fig. 2.16(a)-(c)). This GB behaviour was characterised by more stochastic shear stress and GB motions, and the coupling factor was lower than that for the first starting configuration (SC-1) at the same temperature. The third type of GB behaviour referred to the mechanisms of slowly-move and quickly-go, and the direction of the GB motion was opposite to the direction in the previous two types (Figs. 2.16(c) and (d)). Also, the coupling factor was much higher than the factors in the previous two types. Different GB structures were revealed to be responsible for various GB behaviours.
Niu et al. [53] performed atomistic simulations on a series of [1 0 0] STGBs in BCC W, and found that shear-coupled GB motion occurred via two modes of dislocation movement (\(<1\ 0\ 0>\) and \(<1\ 1\ 0>\) directions) based on GB structure. It
was surprising to find that an unusual tilt axis-orientated atomic shuffling can facilitate shear-coupled GB motion following the <1 1 0> mode. As shown in Fig. 2.17, seven GBs (marked by a dashed circle in the figure), which were supposed to operate in the <1 1 0> mode, were actually in the region of the <1 0 0> mode with a high critical stress. As expected, there was no atomic shuffling for GBs operating in the <1 0 0> mode, while atomic shuffling occurred for all GBs in the <1 1 0> mode. In order to further explain this observation, the GB motions of the \( \Sigma 97 (0 5 \bar{1}3) \) symmetric tilt GB at 0.1 K and 300 K were studied. The results showed that at 0.1 K, the \( \Sigma 97 (0 5 \bar{1}3) \) GB moved in the <1 0 0> mode, whereas the mode of GB motion changed when the temperature was increased to 300 K. The main reason was that high temperatures induced structural transformation and increased atomic shuffling along the tilt axis.

![Critical stress, SCM mode and whether tilt axis-oriented atomic shuffling exists for the SCM process of the [100] group STGBs at 0.1 K.](image)

To obtain a greater understanding of SCM in BCC metals, Niu et al. [54] investigated the \( \Sigma 13 [1 0 0] (0 1 \bar{5}) \) and \( \Sigma 85 [1 0 0] (0 7 \bar{6}) \) GBs in BCC W, and found that the shear strength and thermal resistance of the <1 0 0> model GBs were higher than those of the <1 1 1> models. In other words, the dislocations of the <1 0 0> GBs were more difficult to glide than the dislocations of the \( \frac{1}{2}<1 1 1> \) GBs. As shown in Fig. 2.18 (a)-(f), the migration of the \( \Sigma 85 \) GB was significantly
suppressed by low temperatures. In addition, as shown in Fig. 2.18 (g)-(i), half-jump probability increased with rises in temperature. In general, after the first half jump, elastic energy was released, and this was accompanied by a second, or even multiple, half jumps at relatively high velocities.  

Fig. 2.18 Shear stress and GB displacements as a function of time for the $\Sigma 85$ and $\Sigma 13$ GBs. [54]  

Huang et al. [55] performed MD simulations of the $\Sigma 5 <0 0 1> \{3 1 0\}$ symmetric tilt GB in BCC Nb to study the shear behaviours of the GBs. They found that the coupled motion, which was associated with the GB sheared along $[1 \bar{3} 0]$, decreased exponentially with increasing temperature, as shown in Fig. 2.19. For the GBs shearing along $[0 0 \bar{1}]$, pure sliding behaviour was observed in most temperature conditions, except for 1 K. For the GBs shearing between $[1 \bar{3} 0]$ and $[0 0 \bar{1}]$, the GB presented coupled motion behaviour similar to the $[1 \bar{3} 0]$ direction when the shear angles between the shear directions and the tilt axes were larger than a certain value.
2.6 Summary

From the literature review conducted in this chapter, it has been concluded that atomistic simulations can provide a wealth of information about GBs, including information about GB structures, GB energies and plastic deformation mechanisms such as GB sliding, shear-coupled GB motion, and the dislocation nucleation of GBs. Although previous studies have provided insights into these related GB properties, most research has focused primarily on GBs with $<0 \ 0 \ 1>$, $<1 \ 1 \ 0>$ and $<1 \ 1 \ 1>$ tilt axes, and the range of misorientation angles and tilt axes studied has been limited. In this thesis, GBs with a series of tilt axes and misorientation angles have been simulated. Specifically, the GB structure for each simulation case was identified and the corresponding GB energies were calculated, and the relationship between GB structure and energy was analysed. Moreover, detailed investigations of dislocation nucleation from GB were carried out.
Chapter 3

Research methodology

3.1 Introduction

This thesis conducted atomistic simulations to investigate the structures and properties of GBs. Two main types of atomistic simulations, molecular statics (MS) simulations and molecular dynamics (MD) simulations, were carried out using the parallel molecular dynamics code LAMMPS with the embedded-atom method (EAM) potentials. MS calculations employ numerical optimisation techniques to minimise the potential energy of the system at 0 K. In contrast, MD simulations use atomic coordinates with atomic velocities to incorporate the effects of temperature into the system.

In previous research work, bicrystal systems have been proven to be able to allow a more controlled investigation of GB properties. Therefore, this thesis took full advantage of the bicrystal model to investigate the mechanical properties and deformation mechanisms of GBs. The visualisation tool, Ovito, was used to illustrate the structures of the simulated bicrystal models. The Crystal Analysis Tool developed by Stukowski [56] was used to detect dislocations.

3.2 Molecular dynamics simulations

In this thesis, MD simulations were used to study the dislocation nucleation mechanisms of GBs at the nanoscale. MD simulations are based on Newton's second law of motion:
\[ \dot{p}^i = m v^i \quad \text{(3-1)} \]

where

\[ \dot{r}^i = \frac{dr^i}{dt} = \frac{p^i}{m} \quad \text{(3-2)} \]

Here, \( m \) presents the mass of an atom, \( p^i \) shows the momentum and \( v^i \) is the velocity of the \( i^{th} \) atom, \( r^i \) represents the atomic position vector for the \( i^{th} \) atom, and the ‘dot’ signifies the first derivative with respect to time. The most widely-used method to solve Eqns. (3-1) and (3-2) in molecular dynamics is the Velocity Verlet finite-difference algorithm [57]. This algorithm has many desirable properties because its form is exactly time reversible (which allows the equations of motion to be propagated forward in time without iteration) and symplectic (the volume in phase space is conserved), ensuring long simulation time stability and convergence [58]. Also, the Velocity Verlet algorithm is efficient as it only requires one force evaluation per time step. The formulae used in the Velocity Verlet algorithm are expressed as follows:

\[ v^i \left( t + \frac{\Delta t}{2} \right) = v^i(t) + \frac{\Delta t}{2m} F^i(t) \quad \text{(3-3)} \]

\[ r^i(t + \Delta t) = r^i(t) + \Delta t v^i(t + \frac{\Delta t}{2}) \quad \text{(3-4)} \]

\[ v^i(t + \Delta t) = v^i \left( t + \frac{\Delta t}{2} \right) + \frac{\Delta t}{2m} F^i(t + \Delta t) \quad \text{(3-5)} \]

where \( \Delta t \) is the time step for the MD simulation, which is typically in the order of femtoseconds. In the Velocity Verlet algorithm, the velocity of each atom is first calculated at a half time step forward using the current value of the atomic forces. Then, the atomic positions are updated to \( t + \Delta t \) using the values of the atomic velocities at the half time step. Next, a force calculation is performed using the
updated atomic positions. Finally, the atomic velocities are evolved to the full time step using the updated force vector.

After the starting configuration has been defined, the motions’ equations are iterated by physical time until the system has reached final thermal equilibrium. Sometimes, if one wants to prescribe a certain value for the equilibrium temperature in advance, this can be done by re-scaling the velocities for the equilibration of the MD model, or by using more elegant methods such as the constant volume canonical (NVT), and the isobaric-isothermal canonical (NPT) to keep the temperature constant.

3.3 Molecular statics

In this thesis, molecular statics (MS) is applied to compute the minimum energy interface structures and excess energies. The conjugate gradient (CG) method [59] may be used to find the minimum of any continuous function \( f(x) \) provided \( f'(x) \) contains a lower bound and the gradient \( f'(x) \) can be computed. The procedure of energy minimisation is as shown in Fig. 3.1.
CG is a prominent iterative technique used in this thesis to solve sparse systems of equations. Eqn. (3-6) defines the force vector, which is the negative gradient of potential energy $U$. The minimum potential energy can be found through setting the gradient equal to zero and then solving for the appropriate values of $r_N$.

\[
g_m = -\frac{\partial U(r_N)}{\partial r_m}
\]  \hspace{1cm} (3-6)

\[
r_{m+1} = r_m + \alpha_m d_m
\]  \hspace{1cm} (3-7)

\[
[U'(r_m + \alpha_m d_m)]^T d_m = 0
\]  \hspace{1cm} (3-8)
In Eqn. (3-7), \(d_m\) is the step (or search) direction and \(\alpha\) is a scalar that minimises potential energy in the search direction. It is noted that \(d_m\) is not typically a unit vector. In general, the solution for \(\alpha\) requires that the gradient of the potential energy at point \(r_m + \alpha_m d_m\) be orthogonal to the search direction (Eqn. (3-8)).

### 3.4 Potential energy

The choice of inter-atomic potential determines the accuracy of MC and MD simulations. Daw and Basked [60, 61] developed the embedded-atom method (EAM) to illustrate atomic bonding in an FCC metallic system. To approximate the potential energy of a group of atoms \(U\), EAM includes both pair interactions between nuclei of atoms \(i\) and \(j\) and the embedding energy as a function of the local background electron density around the \(i^{th}\) atom.

\[
U = \sum_i G^i \left( \rho^i_{\text{ave}}(r^{ij}) \right) + \frac{1}{2} \sum_{i,j} \phi(r^{ij})
\]  

(3-7)

where \(G^i\) is the embedding energy function, \(\rho^i_{\text{ave}}\) is the spherically averaged background electron density because of neighbouring the atom \(i^{th}\), \(\phi\) is the pair interaction and \(r^{ij}\) presents the distance between atoms \(i\) and \(j\). Johnson et al. [60] pointed out that the embedding energy depends on the local background electron densities, which are calculated using linear superpositions of the densities from neighbouring atoms (Eqn. (3-8)).

\[
\rho^i_{\text{ave}}(r^{ij}) = \sum_{j \neq 1} \rho^j_{\text{ave}}(r^i - r^j)
\]  

(3-8)

EAM potential [62] has many advantages in representing the atomic interplay. For instance, at the surface of a crystal, the atomic bonds may have different properties than in the bulk, and the EMA potentials are able to capture these effects. This characteristic is particularly important for metals. EAM has been
shown to be an effective way of conducting MD simulations of FCC crystal (Ni, Cu, Al et al.) [63-68]. EMA potential can predict stable stacking fault energies (SFE), which are critical for atomistic fracture and deformation simulations. Rice [69] found that EAM potentials can also be applied to predict dislocation nucleation events. In this thesis, the EAM potentials developed by Mishin et al. [70] are used to describe inter-atomic interactions in MC and MD simulations for Cu and Al.

### 3.5 MC and MD simulation code LAMMPS

In this thesis, all calculations were carried out using the parallel molecular dynamics code LAMMPS, as shown in Affiliation II. LAMMPS is a classical MC and MD code designed for parallel computing. It has potential for research into solid, liquid or gaseous state materials, and can also be used to model atomic, polymeric, biological, metallic, granular and coarse-grained systems under different force fields and boundary conditions. Moreover, it is easy to modify or extend. For efficiency of computing, LAMMPS uses neighbour lists to track nearby particles. These lists are optimised for particle systems that repel at short distances. Therefore, the local density of particles never becomes too large. For parallel computing, LAMMPS uses the technique of spatial decomposition to partition the simulation domain into small 3D sub-domains, one of which is assigned to each processor. Processors communicate and store ‘ghost’ atom information for atoms that border their sub-domains.

### 3.6 Visualisation tool

After the MD simulations, the visualisation tool, Ovito, was used to visualise atomistic configurations. Ovito [56, 71] provides numerous flexible functions to identify and accentuate the characteristics of certain structures of atomistic
configurations. Firstly, the coordination numbers of the atoms are computed automatically and can be used for colour encoding. Atoms with certain coordination numbers can be easily made invisible, and only the crystalline defects can be rendered. Secondly, the local atomic strain can be computed and displayed. Thirdly, an initial configuration can be dyed in Ovito, and then the coloured atoms can be tracked in subsequent configurations. This function is very useful for visualising diffusions and/or deformations induced by atomic displacements. Users can save an arbitrary set of calculated results of atomic properties, including kinetic energies, potential energies, local atomic modules and local atomic stresses.

3.7 Common neighbour analysis

The common neighbour analysis (CNA) [72, 73] technique is widely applied to identify defect structures and evolution in the simulation processes. This method provides a classification of all atoms through their local crystallinity. CNA selects common neighbours from a pair of atoms, which are separated by less than the second-nearest neighbour distance, and then introducing a classification scheme for the nearest-neighbour bond pathways of the two atoms. Currently, there are five kinds of CNA patterns: (1) FCC=1, (2) HCP=2, (3) BCC=3, (4) icosohedral=4, (5) unknown=5 and 0 for atoms not in the specified computing group.

3.8 Dislocation extraction algorithm

The dislocation extraction algorithm (DXA) uses features of the Burgers circuit test, including constructions of the closed paths around the defects of dislocations and illustrations of the perfect crystal lattices to compute the Burgers vector [74, 75]. The advantages of the DXA are that the Burgers circuit procedure is independent
of a structure’s dislocation core details, and it always yields the true Burgers vectors of the dislocations; furthermore, previous knowledge of possible dislocation types is not required.

3.9 Summary

This chapter introduced the basic theories for MD simulation, MS simulation and EAM potential, and basic information for the visualisation method, common neighbour analysis (CNA) and the dislocation extraction algorithm used in the present thesis. MD and MS are used to study dislocation activities and GB energy, respectively. The CNA technique is applied in analysing the defects of GB structures and their evolution during the simulation. The DXA is used to analyse dislocation movements and reactions.
Chapter 4

Grain boundary structure and grain boundary energy

4.1 Introduction

According to Sutton et al. [76], the coherency of high-angle boundaries can be described using the structural unit model (SUM). Coincident site lattice (CSL) methodology has been applied in this thesis to analyse the structures of GBs. CSL notation is an important tool to characterise GB structures because the patterns of CSL lead directly to definable periodic structures at the GBs.

Sutton et al. [76] conducted atomistic simulations with a pair-potential function to show that the interfaces of FCC bicrystal metals may be viewed as a linear combination of ‘structural units’ (SUs). For the $<0 0 1>$ tilt axis, Wang et al. [77] found that the favoured boundaries were the $\Sigma 1 (1 1 0)$ GB (perfect lattice), $\Sigma 5 (2 1 0)$ GB, $\Sigma 5 (3 1 0)$ GB and the $\Sigma 1 (1 0 0)$ GB (perfect lattice). The SUs have been defined as A-D in Reference. [77], respectively. The $\Sigma 5$ GB is the lowest-order $\Sigma$ boundary for the $<0 0 1>$ tilt axis. However, Sutton et al. [76] found that the favoured interfaces sometimes did not correspond to the lowest $\Sigma$ value for a given tilt axis. For the $<1 \overline{1} 0>$ tilt axis, they proposed that the favoured boundaries existed in the $\Sigma 27 (1 1 5)$ GB and $\Sigma 11 (1 1 3)$ GB. Rittner et al. [23] evaluated the entire range of the $<1 \overline{1} 0>$ tilt axis and found that the favoured boundaries were the $\Sigma 1 (0 0 1)$ GB (perfect lattice), $\Sigma 27 (1 1 5)$ GB, $\Sigma 11 (1 1 3)$ GB, $\Sigma 3 (1 1 1)$ GB, $\Sigma 9 (2 2 1)$ GB and the $\Sigma 1 (1 1 0)$ GB (perfect lattice). The SUs
associated with the boundaries mentioned above were defined as A-E in Refs. [23], respectively.

In this chapter, simulations of bicrystal GBs and minimal GB energies are the main research projects. Applying the MS simulation method, 1184 GB models were simulated, including STGBs and ATGBs. After the procedure of GB energy minimisation, this part is trying to illustrate the relationship between minimal GB energy and misorientation angles and tilt axes.

4.2 Simulation model

Fig. 4.1 shows the bicrystal symmetric tilt GB model used in the present study. Two identical crystals with the same orientation were first generated. One crystal (the lower grain in Fig. 4.1) was then rotated around the tilt axis by $\theta/2$ (where $\theta$ is the misorientation angle) in a clockwise direction, while the other crystal (the upper grain in Fig. 4.1) was rotated around the same axis by $\theta/2$ in an anticlockwise direction. The GB plane was set parallel to the X-Y plane such that the first crystal formed the lower grain and the second crystal formed the upper grain. The Miller indices of the tilt axes in the locale crystallographic systems of both grains were the same. The Miller indices of the GB plane in the locale crystallographic systems of the upper grains and lower grains are denoted by $(m \ n \ l)_u$ and $(m \ n \ l)_l$ respectively. The influence of the size of the bicrystal model has been considered in this thesis. In order to minimise the effect of model size on GB energy, the length of the Y direction of the models must be sufficiently long. In this thesis, the dimensions of the simulation model were about $140\AA \times 280\AA \times 140\AA$ ($X \times Y \times Z$) for both Cu and Al. The total numbers of atoms are
approximately 500,000 and 300,000 for the Cu and Al simulation models respectively.

![Bicrystal symmetric tilt GB model](image)

**Fig. 4.1** Bicrystal symmetric tilt GB model

A total of 1184 GB cases (446 STGBs and 738 ATGBs), with various tilt axes and orientation angles, were simulated. Sixty-six tilt axes, as marked by dots in the stereographic triangle in Fig. 4.2, were used. The Miller indices of all the tilt axes are listed in Table 4.1. Their GB structures and energies are discussed in Section 4.3 and Section 4.4.

For the GBs tilted about the axes of [0 0 1], <0 n l> and <m m l>, the misorientation angles varied from 0° to 90°. For the GBs tilted about the axes of [1 1 0] and <m n l>, the misorientation angles ranged from 0° to 180°. For the GBs tilted about the axis of [1 1 1], the misorientation angles varied from 0° to 60°. Both Cu and Al were modelled using EAM potential. The periodic boundary conditions in the simulation models were applied in three directions. The periodic boundary conditions in the X and Z directions gave an infinite GB plane between the upper grain and the lower grain to eliminate the effects of the free surface, while the periodic boundary condition in the Y direction introduced a second GB plane at the periodic border and the two boundaries had identical structures.
Table 4.1 Miller indices of the tilt axes used in the simulations

<table>
<thead>
<tr>
<th>General form</th>
<th>Miller index</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0 0 1]</td>
<td>[0 0 1]</td>
</tr>
<tr>
<td>[1 1 0]</td>
<td>[1 1 0]</td>
</tr>
<tr>
<td>[1 1 1]</td>
<td>[1 1 1]</td>
</tr>
<tr>
<td>&lt;0 n l&gt;</td>
<td>[0 1 2], [0 1 3], [0 1 4], [0 1 5], [0 1 10]</td>
</tr>
<tr>
<td>&lt;m m l&gt;</td>
<td>[1 1 2], [1 1 3], [1 1 5], [1 1 7], [2 2 1], [2 2 3], [2 2 5], [3 3 1], [4 4 5], [5 5 1], [5 5 4]</td>
</tr>
<tr>
<td>&lt;m n l&gt;</td>
<td>[1 2 3], [1 2 4], [1 2 5], [1 2 7], [1 2 9], [1 2 15], [1 3 4], [1 3 5], [1 3 6], [1 3 7], [1 3 9], [1 3 12], [1 3 15], [1 4 6], [1 4 7], [1 5 6], [1 5 7], [1 5 10], [1 5 13], [1 6 10], [1 8 12], [1 10 11], [1 10 13], [2 3 4], [2 3 5], [2 3 6], [2 3 7], [2 3 9], [2 4 5], [2 4 7], [2 5 6], [2 6 7], [2 9 10], [3 4 5], [4 5 6], [4 5 7], [4 5 8], [4 5 9], [4 6 7], [4 8 9], [7 8 9]</td>
</tr>
</tbody>
</table>

Fig. 4.2 Stereographic triangle showing 66 crystallographic orientations of the tilt axes

The GB energy, denoted by $\gamma_{GB}$, was calculated using Eqn. (4-1), where $E$ represents the total potential energy of all the atoms in the simulated domain after energy minimisation. $E_{\text{atom}}$ is the potential energy of a single atom in the perfect Cu lattice (-3.54eV) or Al lattice (-3.36eV). $N$ is the number of atoms in the simulated domain, and $A$ indicates the area of the GB plane.
\[
\gamma_{GB} = \frac{E - N \cdot E_{atom}}{2A}
\]  

(4-1)

The simulation details for energy minimization have been given in the thesis as described below: molecular statics calculations with a nonlinear conjugate gradient algorithm are used to refine the initial GB structures. Periodic boundary conditions in the simulation models were applied in all direction. The energy minimization calculations were performed at 0K. Performing energy minimization calculations over the entire range of GBs using the Mishin EAM potential for Cu and Al. After two times energy minimization procedures, the minimum GB energy has been calculated, the Lammps code of “energy minimization” was shown in Affiliation III. After attaining minimum energy configuration, the simulation model was equilibrated using MD in the isobaric-isothermal (NPT) ensemble at a pressure of 0 bar and a temperature of 0K.

4.3 Structures and energies of symmetric tile GBs

In this thesis, 446 models of the STGBs were used to investigate GB energy and the characteristics of GB structures.

4.3.1 Structures and energies of STGBs with the tilt axis of [0 0 1]

The simulated GB energies for twenty-eight cases with the same tilt axis of [0 0 1] and different misorientation angles \( \theta \) are listed in Table 4.2.

<p>| ( \Sigma ) value | Misorientation angle ( \theta ) ((^\circ)) | GB plane in upper Grain (m n l)(_u) | GB plane in lower Grain (m n l)(_l) | GB energy (mJ/m(^2)) | Cu | Al |
|-------------------|----------------------|----------------------------|----------------------------|----------------------|-------------------|
| ( \Sigma 401 )   | 5.7                   | (20 1 0)                  | (20 -1 0)                  | 470                  | 302               |     |
| ( \Sigma 197 )   | 8.2                   | (14 1 0)                  | (14 -1 0)                  | 578                  | 362               |     |</p>
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<th>Σ</th>
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<th>11.4</th>
<th>(10 1 0)</th>
<th>(10 -1 0)</th>
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<th>419</th>
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<td>(9 -2 0)</td>
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<td>499</td>
<td></td>
</tr>
<tr>
<td>Σ17</td>
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<td>(4 -1 0)</td>
<td>915</td>
<td>486</td>
<td></td>
</tr>
<tr>
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<td>(7 -2 0)</td>
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<td>497</td>
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<td>(7 -4 0)</td>
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<td>(4 -3 0)</td>
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<td>(5 -4 0)</td>
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<td>(6 -5 0)</td>
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</table>
The relationships between the misorientation angle and GB energy for Cu and Al are shown in Fig. 4.3. It can be seen that the GB energies of Cu are approximately twice as high as those of Al. The $\Sigma 97$ GBs with the misorientation angle of 50.4° at both curves have the maximum GB energies of 984mJ/m$^2$ for Cu and 529mJ/m$^2$ for Al. The local minimum GB energies correspond to two $\Sigma 5$ GBs, namely $\Sigma 5 (3 1 0)$ GB and $\Sigma 5 (2 1 0)$ GB. The GB energy of the $\Sigma 5 (3 1 0)$ GB is lower than that of the $\Sigma 5 (2 1 0)$ GB.

Fig. 4.4 compares the GB energies calculated in the present study with the results published by Mishin et al. [78] for the Cu STGBs with a tilt axis of $[0 0 1]$ and various orientation angles. It can be seen that the two sets of results are in excellent agreement.
Fig. 4.3. GB energy of Cu and Al as a function of the misorientation angle for the GBs with [0 0 1] tilt axes.

Fig. 4.4 GB energy as a function of the orientation angles $\theta$ for the Cu STGBs with [0 0 1] tilt axes compared with the results reported by Mishin et al. [78].

Fig. 4.5 shows the STGB structures of 16 Cu simulation cases selected from Table 4.2. Their orientation angles vary from 5.7° to 83.3°. Snapshots of the atomic configurations of the STGBs were taken after the energy minimisation procedure at 0 K. The black and white dots in Fig. 4.6 represent the atoms at the two adjacent atom layers along the tilt axis.

It can be seen in Fig. 4.5 that all the [0 0 1] tilt GBs are composed of two types of the topologically kite-shaped units, namely E and E$_1$ SUs. However, the distances between the adjacent units or/and the positions of the units relative to the GB plane are different for different misorientation angles. The distance between the adjacent units decreases as the misorientation angle increases until $\theta=53.1^\circ$, as shown in Figs. 4.5 (a)-(k). The GBs for this misorientation range only comprise E SUs, which contains six atoms. When the misorientation angle is greater than 53.1°, the distance between the adjacent units increases with the misorientation angle as shown in Figs. 4.5 (l)-(p). A zigzag boundary plane also exists in the $\Sigma 353$, $\Sigma 233$ and $\Sigma 37$ GB planes with the misorientation angles of 50.4°, 63.2° and 71.1°.
(Fig. 4.5 (j) (l) (m)), respectively. The $\Sigma29$ and $\Sigma97$ GBs with the misorientation angles of 43.6° and 47.9°, as shown in Fig. 4.5 (h) (i), present not only E SUs but also a short-kite-shaped $E_1$ SU, which contains four atoms.
Fig. 4.5. Sixteen STGB structures in Cu with \([0\ 0\ 1]\) tilt axes.

(a) \(\Sigma 401 (20\ 1\ 0)\); (b) \(\Sigma 197 (14\ 1\ 0)\); (c) \(\Sigma 101 (10\ 1\ 0)\); (d) \(\Sigma 37 (6\ 1\ 0)\); (e) \(\Sigma 13 (5\ 1\ 0)\); (f) \(\Sigma 17 (4\ 1\ 0)\); (g) \(\Sigma 5 (3\ 1\ 0)\); (h) \(\Sigma 29 (5\ 2\ 0)\); (i) \(\Sigma 97 (9\ 4\ 0)\); (j) \(\Sigma 353 (17\ 8\ 0)\); (k) \(\Sigma 5 (2\ 1\ 0)\); (l) \(\Sigma 233 (13\ 8\ 0)\); (m) \(\Sigma 37 (7\ 5\ 0)\); (n) \(\Sigma 25 (4\ 3\ 0)\); (o) \(\Sigma 61 (6\ 5\ 0)\); (p) \(\Sigma 145 (9\ 8\ 0)\).

Fig. 4.6 shows eight simulated STGB structures in Al. It can be seen that the GB structures in Al are similar to the GB structures in Cu except for the \(\Sigma 101 (10\ 1\ 0)\) GB with a misorientation angle of 11.4°. The \(\Sigma 101 (10\ 1\ 0)\) GB, as shown in Fig. 4.6 (a), presents an array of long-kite shaped SUs, namely \(E_2\) SU, which has eight atoms in each unit. The \(\Sigma 97 (9\ 4\ 0)\) GB, which has the highest GB energy, contains both \(E\) and \(E_1\) SUs, as shown in Fig. 4.6 (d). Two \(\Sigma 5\) GBs (\(\Sigma 5 (3\ 1\ 0)\) and \(\Sigma 5 (2\ 1\ 0)\) have the local minimum GB energies. Both GBs are composed entirely of \(E\) SUs. The above results seem to indicate that \(E\) SUs have lower GB energies than \(E_1\) SUs. In addition, the zig zag boundary plane is observed in the \(\Sigma 17 (5\ 3\ 0)\) GB (Fig. 4.6 (f)).
Fig. 4.6. Eight GB structures in Al with [0 0 1] tilted axes.
(a) $\Sigma 101$ (1 0 1 0); (b) $\Sigma 13$ (5 1 0); (c) $\Sigma 5$ (3 1 0); (d) $\Sigma 97$ (9 4 0); (e) $\Sigma 5$ (2 1 0); (f) $\Sigma 17$ (5 3 0); (g) $\Sigma 25$ (4 3 0); (h) $\Sigma 145$ (9 8 0).

4.3.2 Structures and energies of STGBs with tilt axes of [1 1 0]

Table 4.3 lists all the simulation cases of Cu and Al with tilt axes [1 1 0] and various misorientation angles ranging from 0° to 180°, which cover all the distinct GB structures for this tilt axis. The simulated GB energies are also given in Table 4.3.

<table>
<thead>
<tr>
<th>$\Sigma$ value</th>
<th>Misorientation angle $\theta$ (°)</th>
<th>GB plane in upper Grain</th>
<th>GB plane in lower Grain</th>
<th>GB energy (mJ/m²)</th>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>Cu</td>
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<td></td>
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<td>Al</td>
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</table>

48
<table>
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<tr>
<th></th>
<th>$(m \ n \ l)_u$</th>
<th>$(m \ n \ l)_l$</th>
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<tr>
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<td>8.1</td>
<td>(1 1 20)</td>
<td>(1 1 -20)</td>
</tr>
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<td>$\Sigma_{73}$</td>
<td>13.4</td>
<td>(1 1 12)</td>
<td>(1 1 -12)</td>
</tr>
<tr>
<td>$\Sigma_{33}$</td>
<td>20.1</td>
<td>(1 1 8)</td>
<td>(1 1 -8)</td>
</tr>
<tr>
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<td>26.5</td>
<td>(1 1 6)</td>
<td>(1 1 -6)</td>
</tr>
<tr>
<td>$\Sigma_{27}$</td>
<td>31.6</td>
<td>(1 1 5)</td>
<td>(1 1 -5)</td>
</tr>
<tr>
<td>$\Sigma_{9}$</td>
<td>38.9</td>
<td>(1 1 4)</td>
<td>(1 1 -4)</td>
</tr>
<tr>
<td>$\Sigma_{57}$</td>
<td>44.0</td>
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<td>(2 2 -7)</td>
</tr>
<tr>
<td>$\Sigma_{11}$</td>
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<td>(1 1 3)</td>
<td>(1 1 -3)</td>
</tr>
<tr>
<td>$\Sigma_{123}$</td>
<td>53.6</td>
<td>(5 5 14)</td>
<td>(5 5 -14)</td>
</tr>
<tr>
<td>$\Sigma_{33}$</td>
<td>59.0</td>
<td>(2 2 5)</td>
<td>(2 2 -5)</td>
</tr>
<tr>
<td>$\Sigma_{171}$</td>
<td>65.5</td>
<td>(5 5 11)</td>
<td>(5 5 -11)</td>
</tr>
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<td>$\Sigma_{3}$</td>
<td>70.5</td>
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<td>$\Sigma_{81}$</td>
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<td>(4 4 -7)</td>
</tr>
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<td>82.9</td>
<td>(5 5 8)</td>
<td>(5 5 -8)</td>
</tr>
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<td>(2 2 -3)</td>
</tr>
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<td>$\Sigma_{17}$</td>
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<td>(3 3 -4)</td>
</tr>
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<td>$\Sigma_{57}$</td>
<td>97.1</td>
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<td>(4 4 -5)</td>
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<td>(7 7 -8)</td>
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<td>(1 1 -1)</td>
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<td>(11 11 10)</td>
<td>(11 11 -10)</td>
</tr>
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<td>$\Sigma_{33}$</td>
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<td>(5 5 -4)</td>
</tr>
<tr>
<td>$\Sigma_{123}$</td>
<td>126.4</td>
<td>(7 7 5)</td>
<td>(7 7 -5)</td>
</tr>
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</table>
Fig. 4.7 shows calculated GB energy as a function of the GB misorientation angle for the STGBs with tilt axes of [1 1 0]. It can be seen that the GB energies of Cu are higher than those of Al. There are three local maximum energy points and two local minimum energy points in both curves. The local maximum energies are located at the misorientation angles of 26.5°, 77.9° and 148.4°. They correspond to the \( \Sigma 19 (1 1 6) \), \( \Sigma 81 (4 4 7) \) and \( \Sigma 27 (5 5 2) \) GBs respectively. The \( \Sigma 11 (1 1 3) \) GB with a misorientation angle of 50.5° and the \( \Sigma 3 (1 1 1) \) GB with a misorientation angle of 109.5° have the local minimum GB energies. These two local GB energy points correspond to simple GB structures.
Fig. 4.7 GB energies of Cu and Al as a function of the misorientation angle for the GBs with [1 1 0] tilt axes.

Fig. 4.8 compares the calculated GB energies of the Cu [1 1 0] tilt GB with the results reported by Zhang et al [79]. It can be seen that the two sets of results are in very good agreement.

Fig. 4.9 shows 15 typical GB structures observed in the simulations with a [1 1 0] tilt axis. The GBs with lower orientation angles ($\theta<109.5^\circ$) have a periodic structure composed of the C and D SUs. The C SU is shown in $\Sigma 11$ (1 1 3) GB (as shown in Fig. 4.9 (c)), and the D SU is shown in $\Sigma 3$ (1 1 1) GB (as shown in Fig. 4.9
(h)). It is worth noting that both the C unit and E₁ unit contain four atoms. The difference between them is that three atoms of the C unit are in one plane and the other atom is in another plane. The Σ₉ (1 1 4) θ=38.9° GB in Fig. 4.9 (a) contains two C SUs and one D SU in each GB structural period. As the misorientation angle increases, the number of C units increases. For example, there are four C units in each GB structural period for the Σ₅₇ GBs with the misorientation angle of 136.0°, as shown in Fig. 4.9 (b).

When the misorientation angle reaches 50.5° (Σ₁₁ GB in Fig. 4.9 (c)), the GB is fully composed of C units. A local minimum GB energy exists at this misorientation angle. As the misorientation angle further increases to 53.6° (Σ₁₂₄), the adjacent periodic structure no longer remains in the same plane. There is an offset between two adjacent periodic structures along the (1 1 1) direction. This results in a D unit located several lattices away from the C units. At the Σ₁₂₃ GB (Fig. 4.9 (d)), there are nine C units and one D unit in each structural period and the D unit is 3.5a away from the C units, where a is the lattice constant. As the misorientation angle further increases, both the number of C units and the direction distance between the D and C units in the periodic structure decreases.

At the Σ₃₃ GB θ=58.6° GB (Fig. 4.9 (e)), each periodic structure consists of three C units and one D unit, and the direction distance along (1 1 1) between the D unit and the three C units is 2a. At the Σ₃ GB θ=70.5° GB (Fig. 4.9 (f)), each periodic structure consists of one C unit and one D unit, and the distance along (1 1 1) between the D and C units is a. When the misorientation angle increases to 56.6° (Σ₁₇ in Fig. 4.9 (g)), the A' unit appears. The A and A' SUs are basic units of the Σ₁ (0 0 1) θ=0° and Σ₁ (1 1 0) θ=180° perfect GBs. A' is identical to the A SU but rotated by 90°. The D unit still exists at the GB and the distance between the D
unit and the A’ unit is still $a$. The $\Sigma 3 \ (1 \ 1 \ 1) \ \theta=109.5^\circ$ GB (Fig. 4.9 (h)) is known as the coherent twin boundary. It is composed entirely of D SUs. This GB has the lowest GB energy, as depicted in Fig. 4.9.

At the misorientation angle of 114.5° ($\Sigma 171$ in Fig. 4.9 (i)), the E unit appears at the GBs with the D units. When the misorientation angle increases further, the number of E units increases with the misorientation angle. At the misorientation angle of 153.5° ($\Sigma 19$ in Fig. 4.9 (n)), the GB structure is composed of one E unit and one A unit. At the misorientation angle of 166.6° ($\Sigma 73$ in Fig. 4.10 (o)), the entire GB is composed of E’ and A’ units. The E SUs are no longer at an angle to one side or the other, but are rotated by 90° and labelled as E’ SUs.
Fig. 4.9. Fifteen GB structures in Cu with tilt axes of [1 1 0].

(a) $\Sigma^9 (1 1 4)$; (b) $\Sigma^{57} (2 2 7)$; (c) $\Sigma^{111} (1 1 3)$; (d) $\Sigma^{123} (5 5 14)$; (e) $\Sigma^{33} (2 2 5)$; (f) $\Sigma^3 (1 1 2)$; (g) $\Sigma^{17} (2 2 3)$; (h) $\Sigma^3 (1 1 1)$; (i) $\Sigma^{171} (1 1 1 1 1 0)$; (j) $\Sigma^{33} (5 5 4)$; (k) $\Sigma^{11} (3 3 2)$; (l) $\Sigma^{291} (11 11 7)$; (m) $\Sigma^9 (2 2 1)$; (n) $\Sigma^{19} (3 3 1)$; (o) $\Sigma^{73} (6 6 1)$.

Fig. 4.10 depicts the typical structures of six Al STGBs with [1 1 0] tilt axes. The SUs at these Al STGBs are similar to those for Cu. However, the effect of the misorientation on their GB structures is slightly different. For example, at the
misorientation angle of 70.5° (Σ3), the GBs of Cu contain C and D units, while the GBs of Al consist entirely of E units.

The Σ11 (1 1 3) θ=50.5° GB, Σ3 (1 1 2) θ=70.5° GB and Σ9 (2 2 1) θ=141.1° GB (Fig. 4.10 (b), (c) and (e)) are composed entirely of C, D and E SUs. The corresponding GB energies are 151mJ/m², 355mJ/m² and 447mJ/m² respectively. Therefore, it can be concluded that the D units induce the lowest GB energies, the C units have slightly higher GB energies, and the E units have the highest GB energies.

![GB structures in Al with tilt axes of [1 1 0]](image)

**Fig. 4.10.** Sis GB structures in Al with tilt axes of [1 1 0]

(a) Σ27 (1 1 5); (b) Σ11 (1 1 3); (c) Σ3 (1 1 2); (d) Σ17 (3 3 4); (e) Σ3 (1 1 1); (f) Σ33 (5 5 4).

4.3.3 Structures and energies of STGBs with the tilt axis of [1 1 1]

Eight STGBs with [1 1 1] tilt axes have been modelled in this thesis, as shown in Table 4.4. The misorientation angle θ varies from 0° to 60.
Table 4.4. Simulated GB energies for STGBs with the same tilt axes of [1 1 1] and different misorientation angles

<table>
<thead>
<tr>
<th>Σ value</th>
<th>Misorientation angle θ (°)</th>
<th>GB plane in upper Grain (m n l)u</th>
<th>GB plane in lower Grain (m n l)l</th>
<th>GB energy (mJ/m²)</th>
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</thead>
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<tr>
<td></td>
<td></td>
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<tr>
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<td>17.9</td>
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<tr>
<td></td>
<td></td>
<td>(1 4 5)</td>
<td>(-1 5 4)</td>
<td>Al</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>419</td>
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<td>Σ21</td>
<td>21.8</td>
<td></td>
<td></td>
<td>775</td>
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<tr>
<td></td>
<td></td>
<td>(1 3 4)</td>
<td>(-1 4 3)</td>
<td>450</td>
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<td>Σ13</td>
<td>27.8</td>
<td></td>
<td></td>
<td>842</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2 5 7)</td>
<td>(-2 7 5)</td>
<td>471</td>
</tr>
<tr>
<td>Σ39</td>
<td>32.2</td>
<td></td>
<td></td>
<td>889</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2 3 5)</td>
<td>(-2 5 3)</td>
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<td>Σ7</td>
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<td>867</td>
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<td></td>
<td></td>
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<td>(-1 3 2)</td>
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<td>Σ19</td>
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<td>852</td>
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<td></td>
<td></td>
<td>(3 4 7)</td>
<td>(-3 7 4)</td>
<td>469</td>
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<tr>
<td>Σ37</td>
<td>50.6</td>
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<td>822</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>469</td>
</tr>
<tr>
<td>Σ3</td>
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<td>(1 1 -2)</td>
<td>(-1 2 -1)</td>
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<tr>
<td></td>
<td></td>
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<td>385</td>
</tr>
</tbody>
</table>

The GB energies of STGBs of Cu and Al with [1 1 1] tilt axes as a function of the misorientation angles are shown in Fig. 4.11. Similar to the cases with [0 0 1] and [1 1 0] tilt axes, the GB energies of Cu are much higher than those of Al. The minimum GB energies correspond to the minimum GB energies for the Σ3 (1 1 2)θ=60° GB. They have values of 688mJ/m² for Cu and 385mJ/m² for Al. These minimum GB energies are lower than those with [1 0 0] tilt axes, but much higher than those with [1 1 0] tilt axes.

Fig. 4.12 shows six GB structures of Cu with [1 1 1] tilt axes and different misorientation angles. It is noted that the atomic arrangements at these GBs still demonstrate regularity. However, the GB structures cannot be described by the SUs as performed in Section 4.3.1 and Section 4.3.2. The general trend in the effect of the misorientation angle is that the periodical structure becomes shorter.
as the misorientation angle increases. The GB structures of Al with [1 1 1] tilt axes, which are not shown in this section, are similar to those of Cu.

Fig. 4.11 GB energies of Cu and Al as a function of the misorientation angle for GBs with [1 1 1] tilt axes.

Fig. 4.12. Six GB structures in Cu with tilt axes of [1 1 1]. The green atoms represent FCC atoms, the yellow represent OTHER atoms, and the red atoms represent HCP atoms.
(a) $\Sigma 331 (1 5 6)$; (b) $\Sigma 21 (1 4 5)$; (c) $\Sigma 13 (1 3 4)$; (d) $\Sigma 39 (2 5 7)$; (e) $\Sigma 7 (1 2 3)$; (f) $\Sigma 19 (2 3 5)$. 
4.3.4 Structures and energies of GBs with \(<0 n l>\) tilt axes

There are nine groups of STGBs with \(<0 n l>\) tilt axes modelled in this thesis. The tilt axes are shown in Table 4.5 and the misorientation angles vary from 0° to 90° for each tilt axis. The values of the minimum GB energies are listed in Table 4.5.

<table>
<thead>
<tr>
<th>No.</th>
<th>Tilt axes</th>
<th>Minimum GB energy (mJ/m²)</th>
<th>No.</th>
<th>Tilt axes</th>
<th>Minimum GB energy (mJ/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td></td>
</tr>
<tr>
<td>1</td>
<td>[0 1 2]</td>
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<td>319</td>
<td>6</td>
<td>[0 2 3]</td>
</tr>
<tr>
<td>2</td>
<td>[0 1 3]</td>
<td>699</td>
<td>400</td>
<td>7</td>
<td>[0 2 5]</td>
</tr>
<tr>
<td>3</td>
<td>[0 1 4]</td>
<td>722</td>
<td>457</td>
<td>8</td>
<td>[0 3 4]</td>
</tr>
<tr>
<td>4</td>
<td>[0 1 5]</td>
<td>568</td>
<td>368</td>
<td>9</td>
<td>[0 7 8]</td>
</tr>
<tr>
<td>5</td>
<td>[0 1 10]</td>
<td>564</td>
<td>354</td>
<td></td>
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</tr>
</tbody>
</table>

The GB energies of STGBs of Cu and Al with [0 1 2] and [0 2 3] tilt axes as a function of the misorientation angle are shown in Fig. 4.13. The local maximum energies are located at the misorientation angles of 60.3° and 55.3° respectively. They correspond to the \(\Sigma 2023 (51 34 17)\) and \(\Sigma 2353 (39 24 16)\) GBs respectively.
Fig. 4.13 GB energies of Cu and Al as a function of the misorientation angle for the GBs for [0 1 2] and [0 2 3] tilt axes.

SUs can be observed in some simulation cases. Fig. 4.14 shows two GB structures composed of SUs in Cu and Al with tilt axes of <0 n l>. It can be seen in Fig. 4.14 (a) that the A SUs present in the Cu $\Sigma 2023$ (51 -34 17) $\theta=60.23^\circ$ GBs are tilted at [0 1 2]. The E’ SUs present in Cu $\Sigma 11$ (6 6 4) $\theta=70.53^\circ$ GB are tilted at [0 2 3] (Fig. 4.14 (b)).

![GB Structures](image)

(a) $\Sigma 2023$ (-51 -34 17); (b) $\Sigma 11$ (-6 -6 4).

4.3.5 Structures and energies of STGBs with <m m l> tilt axes

Twelve groups of STGBs with <m m l> tilt axes have been modelled in this thesis. The tilt axes are shown in Table 4.6 and the misorientation angles vary from 0° to 90° for each tilt axis. The minimum GB energies are listed in Table 4.6 as well.

<table>
<thead>
<tr>
<th>No.</th>
<th>Tilt axes</th>
<th>Minimum GB energy (mJ/m$^2$)</th>
<th>No.</th>
<th>Tilt axes</th>
<th>Minimum GB energy (mJ/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
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<td></td>
<td></td>
<td>Cu</td>
</tr>
<tr>
<td>1</td>
<td>[1 1 2]</td>
<td>917</td>
<td>7</td>
<td>[2 2 5]</td>
<td>926</td>
</tr>
<tr>
<td>2</td>
<td>[1 1 3]</td>
<td>943</td>
<td>8</td>
<td>[3 3 1]</td>
<td>698</td>
</tr>
<tr>
<td>3</td>
<td>[1 1 5]</td>
<td>954</td>
<td>9</td>
<td>[3 3 2]</td>
<td>691</td>
</tr>
<tr>
<td>4</td>
<td>[1 1 7]</td>
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<td>10</td>
<td>[4 4 5]</td>
<td>810</td>
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<tr>
<td>5</td>
<td>[2 2 1]</td>
<td>797</td>
<td>11</td>
<td>[5 5 1]</td>
<td>558</td>
</tr>
</tbody>
</table>

59
The GB energies of STGBs of Cu and Al with [1 1 3] and [5 5 1] tilt axes as a function of the misorientation angles are shown in Fig. 4.15. The local maximum energies are located at the misorientation angles of 50.7° and 50.9°, respectively. They correspond to the Σ15 (2 5 1), Σ2353 and Σ69 (8 7 5) GBs respectively.

Fig. 4.15 GB energies of Cu and Al as a function of the misorientation angle for the GBs for [1 1 3] and [5 5 1] tilt axes.

SUs can be observed in some simulation cases. Fig. 4.16 shows four GB structures composed of SUs in Cu and Al with tilt axes of <m m l>. It can be seen in Fig. 4.16 that C SUs are present in Cu Σ2023 (2 5 1) θ=50.7° GBs tilted with [1 1 3] (Fig. 4.16 (a)), and in Cu Σ11 (8 7 5) θ=50.9° GB tilted with [5 5 1] (Fig. 4.16 (b)).

Fig. 4.16 Two GB structures in Cu and Al tilted with <m m l>. The green atoms represent FCC atoms and the yellow atoms represent OTHER atoms.
(a) Cu Σ15 (-2 5 -1); (b) Al Σ69 (8 -7 -5).
4.4 Structures and energies of ATGBs

Besides the 25 groups of STGB structures studied in Section 4.3, 41 groups of ATGB models have been simulated in this thesis. The 41 tilt axes are listed in Table 4.7.

<table>
<thead>
<tr>
<th>No.</th>
<th>Axes</th>
<th>No.</th>
<th>Axes</th>
<th>No.</th>
<th>Axes</th>
<th>No.</th>
<th>Axes</th>
</tr>
</thead>
</table>

The bicrystal simulation model with an ATGB is shown in Fig. 4.17. The crystallographic orientations of the lower grains along the X, Y and Z directions were set up first. For example, for the cases with [1 2 3] tilt axes, the lower grains have crystallographic orientations of [511], [100 11] and [123] along the X, Y and Z directions, respectively. The crystallographic orientation of the upper grain is determined by

\[ r' = R \times r \]  

(4-2)

where

\[ R = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \]  

(4-3)
Here, \( r \) is a matrix of the crystallographic orientations of the lower grains along the X, Y and Z directions, \( r' \) is a matrix of the crystallographic orientations of the upper grain along the X, Y and Z directions, and \( \theta \) is the misorientation angle.

\[ \text{Fig. 4.17 Bicrystal model with asymmetric tilt GB} \]

4.4.1 The analysis of ATGBs with tilt axes \(<121>\>

The calculated GB energies for Cu and Al ATGBs with six \(<121>\>\) tilt axes and 18 misorientation angles are listed in Table 4.8. The maximum energy and minimum energy of each tilt axis are also shown in the table. The maximum and minimum energies for the whole table are 2092mJ/m\(^2\) and 307mJ/m\(^2\) respectively.

<table>
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<tr>
<th>Rotation (°)</th>
<th>[1 2 3]</th>
<th>[1 2 4]</th>
<th>[1 2 5]</th>
<th>[1 2 7]</th>
<th>[1 2 9]</th>
<th>[1 2 15]</th>
</tr>
</thead>
<tbody>
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<td>Al</td>
<td>Cu</td>
<td>Al</td>
<td>Cu</td>
<td>Al</td>
</tr>
<tr>
<td>10°</td>
<td>530</td>
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<td>520</td>
<td>307</td>
<td>727</td>
<td>588</td>
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<tr>
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<td>935</td>
<td>532</td>
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<td>731</td>
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<td>1269</td>
<td>1009</td>
<td>640</td>
<td>994</td>
<td>554</td>
</tr>
<tr>
<td>50°</td>
<td>2092</td>
<td>1229</td>
<td>1101</td>
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</tr>
<tr>
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<td>902</td>
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<td>645</td>
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<td>1007</td>
<td>1261</td>
<td>1009</td>
<td>1167</td>
<td>689</td>
</tr>
</tbody>
</table>
The GB energies of Cu and Al as a function of the misorientation angle for the ATGBs with [1 2 3] and [1 2 4] tilt axes are shown in Fig. 4.18. It can be seen that the misorientation angle significantly affects GB energy. There are several peaks in each of the curves. This phenomenon can also be observed in the curves of other tilt axes.

It is difficult to use the SU method to analyse GB structures for <1 2 l> tilt axes. The SUs only exist in some cases, such as the E unit in Cu ATGB with a tilt axis of [1 2 3], as shown in Fig. 4.19 (a).
Fig. 4.19 Two GB structures in Cu and Al tilted at $<1\ 3\ l>$.

(a) Cu $\sum 21$ (4\ 1\ -2); (b) Al $\sum 13243$ (158\ -1\ -39).

4.4.2 The analysis of the ATGBs with tilt axes $<1\ 3\ l>$

The calculated GB energies for Cu and Al ATGBs with seven $<1\ 3\ l>$ tilt axes and 18 misorientation angles are listed in Table 4.9. The maximum energy and minimum energy of each tilt axis are also shown in the table. The maximum and minimum energies for the whole table are 1955mJ/m$^2$ and 401mJ/m$^2$ respectively.

<table>
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<th>[1 3 5]</th>
<th>[1 3 6]</th>
<th>[1 3 7]</th>
<th>[1 3 9]</th>
<th>[1 3 12]</th>
<th>[1 3 15]</th>
</tr>
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<td>Cu</td>
<td>Al</td>
<td>Cu</td>
<td>Al</td>
<td>Cu</td>
<td>Al</td>
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<td>957</td>
<td>567</td>
<td>1518</td>
<td>988</td>
<td>1169</td>
</tr>
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</table>
The GB energies of Cu and Al as functions of the misorientation angle for the ATGBs with [1 3 4] and [1 3 5] tilt axes as examples are shown in Fig. 4.20. GB energy is apparently affected by the misorientation angle.

Fig. 4.20 GB energies of Cu and Al as functions of the misorientation angle for GBs with [1 3 4] and [1 3 5] tilt axes.

As shown in Fig. 4.21 (a), the $\Sigma 357 (25 5 \overline{8}) \theta=159.3^\circ$ GB presents C and D SUs, but these units are not continuous. The $\Sigma 105 (8 4 \overline{5}) \theta=111.4^\circ$ GB contains C and E SUs.

Fig. 4.21 Snapshot of GBs in Cu and Al tilt with <1 3 l>. The green atoms represented FCC atom, the yellow atoms represented OTHER atom, and the red atoms represented HCP atom.

(a) Al $\Sigma 105 (8 4 -5)$; (b) Cu $\Sigma 357 (25 5 -8)$. 
4.4.3 The analysis of the ATGBs with tilt axes <1 n l>

The current study calculated GB energies for Cu and Al ATGBs with ten <1 n l> tilt axes and 18 misorientation angles, and there are eight groups listed in Table 4.10. The maximum energy and minimum energy for each tilt axis are also shown in the table. The maximum and minimum energies for the whole table are 1333mJ/m² and 449mJ/m² respectively.

<table>
<thead>
<tr>
<th>Rotation axes</th>
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<th>[1 5 10]</th>
<th>[1 5 13]</th>
<th>[1 6 10]</th>
<th>[1 8 12]</th>
<th>[1 10 11]</th>
<th>[1 10 13]</th>
</tr>
</thead>
<tbody>
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<td>Al</td>
<td>Cu</td>
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</tr>
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<td>1040</td>
<td>824</td>
<td>1203</td>
<td>676</td>
</tr>
<tr>
<td>140°</td>
<td>966</td>
<td>745</td>
<td>1008</td>
<td>816</td>
<td>919</td>
<td>753</td>
<td>503</td>
<td>479</td>
</tr>
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<td>150°</td>
<td>1149</td>
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<tr>
<td>160°</td>
<td>997</td>
<td>660</td>
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<td>556</td>
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<tr>
<td>180°</td>
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<td>611</td>
<td>391</td>
<td>1040</td>
<td>577</td>
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</tr>
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<td>611</td>
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<td>Maximum</td>
<td>1149</td>
<td>1023</td>
<td>1313</td>
<td>816</td>
<td>1280</td>
<td>824</td>
<td>1313</td>
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</table>
The GB energy of Cu and Al as a function of the misorientation angle for the ATGBs with [1 5 6] and [1 10 11] tilt axes are shown in Fig. 4.22. The GB energies of Cu are approximately twice those of Al.

![GB energy graphs](image1)

Fig. 4.22 GB energies of Cu and Al as functions of the misorientation angle for GBs with [1 5 6] and [1 10 11] tilt axes.

It is worth noting that the dissociation of GB structures is observed for the $\Sigma 20757$ ($\overline{68} \ 97 \ \overline{62}$) GB in Fig. 4.23 (b). This is due to the asymmetric dissociations of secondary GBs which are associated with Burgers vectors for which Shockley partial dislocations occur. The boundary energy has been lowered by the atomic arrangement of this structure, but it has also created an extra stacking fault area inside the grain.

![GB structure snapshots](image2)

Fig. 4.23 Snapshot of Cu GBs with a tilt of $<1 \ n \ l>$. The green atoms represent FCC atoms, the yellow atoms represent OTHER atoms, the red atoms represent HCP atoms, and blue atoms represent BCC atoms. (a) $\Sigma 147$ (-5 13 -10); (b) $\Sigma 20757$ (-68 97 -62).
4.4.4 The analysis of ATGBs with tile axes \(<2 n \mid l>\)

The calculated GB energies for Cu and Al ATGBs with seven \(<2 n \mid l>\) tilt axes and 18 misorientation angles are listed in Table 4.11. The maximum and minimum energies of each tilt axis are also shown in the table. The maximum and minimum energies for the whole table are 1923mJ/m² and 416mJ/m² respectively.

Table 4.11 the GB energy as a function of rotation axes and misorientation angles

<table>
<thead>
<tr>
<th>Rotation axes (\theta (^\circ))</th>
<th>[2 3 4]</th>
<th>[2 3 7]</th>
<th>[2 4 5]</th>
<th>[2 4 7]</th>
<th>[2 5 6]</th>
<th>[2 6 7]</th>
<th>[2 9 10]</th>
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<td>Al</td>
<td>Cu</td>
<td>Al</td>
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<td>696</td>
<td>727</td>
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<td>662</td>
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<td>Maximum</td>
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<td>1295</td>
<td>1433</td>
<td>373</td>
<td>1769</td>
<td>1335</td>
<td>1923</td>
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</tbody>
</table>

The GB energies of Cu and Al as a function of the misorientation angle for the ATGBs with [2 3 4], [2 6 7], [2 9 10] and [2 4 5] tilt axes are shown in Fig. 4.24.
Fig. 4.24 GB energy of Cu and Al as a function of the misorientation angle for the GBs with the [2 3 4], [2 6 7], [2 9 10] and [2 4 5] tilt axes.

In Fig. 4.25 (a), the $\Sigma 11629 \ (51 \ 62 \ 72) \ \theta = 110.10^\circ$ GB is composed entirely of C SUs. It is difficult to use the SU method to analyse the GB structures for <2 n l> tilt axes.

Fig. 4.25 Snapshot of GBs in Cu and Al with tilt axes of <2 n l>. The green atoms represent FCC atoms, the yellow atoms represent OTHER atoms, and red atoms represent HCP atoms.

(a) Cu $\Sigma 11629 \ (51 \ 62 \ 72)$; (b) Cu $\Sigma 785 \ (-19 \ 18 \ -10)$; (c) Cu $\Sigma 3737 \ (33 \ 56 \ -57)$; (d) Al $\Sigma 7 \ (3 \ 1 \ -2)$. 
4.4.5 The analysis of ATGBs rotated around other axes

The calculated GB energies for Cu and Al ATGBs with eight \(<m n l>\) tilt axes and 18 misorientation angles are listed in Table 4.12. The maximum and minimum energies for each tilt axis are also shown in the table. The maximum and minimum energies for the whole table are 2565mJ/m² and 196mJ/m² respectively.

![Table 4.12](image_url)

Table 4.12: The GB energy as a function of rotation axes and misorientation angles

- **θ (°)**: Rotation angle in degree.
- **GB energy (mJ/m²)**: GB energy for different rotation axes.
- **Cu** and **Al**: GB energies for Cu and Al respectively.

5.0 The GB energy for Cu and Al ATGBs with 8 \(<m n l>\) tilt axes and 18 misorientation angles are listed in Table 4.12. The maximum and minimum energies for each tilt axis are also shown in the table. The maximum and minimum energies for the whole table are 2565mJ/m² and 196mJ/m² respectively.

![Table 4.12](image_url)

**Table 4.12**: The GB energy as a function of rotation axes and misorientation angles

- **θ (°)**: Rotation angle in degree.
- **GB energy (mJ/m²)**: GB energy for different rotation axes.
- **Cu** and **Al**: GB energies for Cu and Al respectively.
The GB energies of Cu and Al as a function of the misorientation angle for ATGBs with [4 5 6] and [7 8 9] tilt axes are shown in Fig. 4.26.

![GB energies of Cu and Al as functions of misorientation angle for ATGBs with [4 5 6] and [7 8 9] tilt axes.](image)

Fig. 4.26 GB energies of Cu and Al as functions of misorientation angle for ATGBs with [4 5 6] and [7 8 9] tilt axes.

In the Fig. 4.27, the arrangement of atoms of GBs presents a certain regularity.

![Al GBs with tilt axes of <m n l>.](image)

Fig. 4.27 Snapshot of Al GBs with tilt axes of <m n l>. The green atoms represent FCC atoms, the yellow atoms represent OTHER atoms, and the red atoms represent HCP atoms.

(a) $\Sigma 17 (-2 -2 3)$; (b) $\Sigma 507 (-19 11 5)$.

### 4.5 Summary

In this chapter MD simulations were conducted to investigate the structures and energies of 446 STGBs and 738 ATGBs of Cu and Al. Sixty-six tilt axes and various misorientation angles (0-180°) have been simulated. After energy minimisation, the characters of GB structures were found to be as follows:

1. The distance between adjacent units changes with misorientation angles in bicrystals with tilt axis of [0 0 1]. To be specific, the minimum GB energy corresponds to the $\Sigma 5 (3 1 0)$ GB which is entirely composed of the E SUs.
2. For the STGBs, the local minimal GB energies were associated with simple GB interface structures. For instance, the $\Sigma 11 \ (1 \ 1 \ 3)$ and $\Sigma 3 \ (1 \ 1 \ 1)$ GBs which are composed entirely of C and D SUs respectively, had local minimal GB energies. On the other hand, for the ATGBs, the GB energies were profoundly affected by their misorientation angles.

3. Periodicity can be observed in the function of GB energy and misorientation angles. This is mainly because of the atomic structures of FCC materials, and it demonstrates that atomic structures have significant effects on material properties.
Chapter 5

Mechanisms of dislocation nucleation from grain boundaries

5.1 Introduction

Studies investigating atomic-scale mechanisms in nanocrystalline materials have progressed remarkably during the last decade. As discussed in Chapter 2, atomistic simulations have been effective in probing GB-mediated plasticity processes, especially for the nucleation of partial dislocations from GBs in a wide range of material systems. Sansoz and Molinari [81] performed extensive MD simulations on bicrystal models in the FCC metals Cu and Al under shear. Yamakov and Van Swygenhoven [57, 64, 82] studied GB behaviours during plastic deformation processes in nanocrystalline FCC metals. It was found that GBs mainly provided the sources for dislocation nucleation when the grain size was below 10 nm. Recently, Spearot et al. [83,84] conducted a series of MD simulations to investigate nucleation events in GBs with <1 0 0> and <1 1 0> tilt axes over a wide range of misorientation angles and found that the tensile stress required for dislocation nucleation was directly correlated to grain orientation and certain structural units of the GBs. Tschopp et al. [30] and Spearot et al. [42] studied the process of dislocation nucleation in bicrystal GBs with dissociated structures. According to their simulation results, the dissociated structures served as sites for dislocation nucleation and promoted nucleation events in secondary
slip systems in GBs. More information about dislocation nucleation events from
the GB plane can be found in Chapter 2.

The main aim of this thesis was to examine the influence of tilt axes and
misorientation angles on the grain boundary structures, and to examine the
nucleation dislocation mechanisms of FCC materials through simulation of tensile
loading. The simulations demonstrated that it was possible to examine the
relationship between the dislocation mechanism and tilt axes and misorientation
angles. Following the simulations, the relationship of stress-strain were analysed,
comparing with the dislocation analysis. These analyses improved our
understanding of the FCC materials’ mechanisms.

There are three main differences between this thesis and previous research.
Firstly, this thesis covers almost all the possible tilt axes and misorientation angles
of FCC materials. Secondly, the stress-strain relationship has been analysed
through tensile loading. Thirdly, GB structures with the lowest GB energies have
been identified using MD simulation, which clearly shows the effects of
nucleation on dislocation during the loading procedure.

In this chapter, the mechanisms of dislocation nucleation of different GBs are
systematically studied at the atomic scale using MD simulations.

5.2 Simulation model

The EAM potential developed by Mishin et al. [61] for Cu and Al were used in this
study. This approach can accommodate a large amount of experimental and first
principles data. The bicrystal model which was used in this study is based on two
separate grains, upper grain and lower grain, with different orientations. The
misorientation angle between the two types of grains is θ, which has a symmetric
tilt with \(<m n l>\). After identifying the lowest possible energy configuration, the system was equilibrated within an isobaric-isothermal (NPT) ensemble at the desired temperature and pressure for 0.1 ns. Tensile deformation was then achieved by uniformly stretching the simulation cell along the Y direction with a certain strain rate. In previous research, \(1 \times 10^{10}, 1 \times 10^9, 1 \times 10^8\) and \(2 \times 10^8\) were widely used in MD simulations [12,29,35,44,47,79,83]. The results of these simulations with different strain rates showed similarity during the stress-strain process, which is characteristic of MD simulation. Therefore, a strain rate of \(2 \times 10^8/s\) was chosen for this thesis. Besides that, this strain rate has slight effects on the structures of GBs.

The deformation process was conducted with two different boundary conditions along the X and Z directions: free and constrained boundary conditions. Free tension boundary conditions allowed the boundaries in the lateral (X and Z) directions to expand/contract to ensuring that transverse stresses are free \((\sigma_{xx} = \sigma_{zz} = 0)\), while the boundaries in the lateral (X and Z) directions are maintained at a zero strain condition \((\varepsilon_{xx} = \varepsilon_{zz} = 0)\) under constrained tension boundary conditions. The periodic boundary condition was applied to the Y direction.

In regard to the mechanical properties, the stress of the system is the average stress of all the atoms, and the strain of the system is derived from the elongation of the simulation domain along the Y direction. In this thesis, the main research focus was grain boundary structures with a series of rotation axes and orientation angles, and their impacts on dislocation nucleation mechanisms. The rotation axes and orientation angles were the only dynamic variables considered during the process of simulation. Other parameters, such as strain rate and temperature, were all defined as theoretical values. Therefore, the temperature of the
simulation was maintained at 1 K and the integration time step was set to 1 fs throughout the MD simulations.

The visualisation tool Ovito [16, 17, 54] was used to illustrate the inner structures of the bicrystal models. The CNA [77] technique was applied to identify structural defects and the process of their evolution during the simulations. The DXA technique [13, 54] was used for computing the Burgers vectors of the GB nucleated dislocations.

5.3 Tensile deformation response of bicrystal models tilt with [0 0 1]

5.3.1 The analysis of stress-strain in GBs with [0 0 1] tilt axes

Fourteen bicrystals with the same [0 0 1] tilt axis and different misorientation angles, as listed in Table 5.1, were subjected to tensile deformation in the Y direction.

Table 5.1 Schmid factor of resolved shear stress on the \{1 1 1\} <1 1 2> slip system for the [0 0 1] tilt GBs.

<table>
<thead>
<tr>
<th>Slip plane</th>
<th>Slip direction</th>
<th>Grain boundary plane (m n l), and misorientation angle (θ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1 1 1)</td>
<td>[1 1 2]</td>
<td>0.312 0.326 0.336 0.347 0.368 0.387 0.398</td>
</tr>
<tr>
<td></td>
<td>[1 Ê 1]</td>
<td>0.178 0.163 0.153 0.139 0.108 0.077 0.057</td>
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<tr>
<td></td>
<td>[2 1 1]</td>
<td>0.491 0.490 0.488 0.485 0.477 0.465 0.455</td>
</tr>
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<td>(1 1 Ê)</td>
<td>[1 1 2]</td>
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<td>0.178 0.163 0.153 0.139 0.108 0.077 0.057</td>
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<td>[2 1 1]</td>
<td>0.491 0.490 0.488 0.485 0.477 0.465 0.455</td>
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<tr>
<td>(1 Ê 1)</td>
<td>[1 1 2]</td>
<td>0.159 0.145 0.136 0.125 0.103 0.084 0.073</td>
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<tr>
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</table>

76
The maximum values of Schmid factor for each grain boundary are shaded.

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<td>[1 2 1]</td>
<td>0.207</td>
<td>0.189</td>
<td>0.177</td>
<td>0.153</td>
<td>0.147</td>
<td>0.127</td>
<td>0.108</td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>[2 1 1]</td>
<td>0.267</td>
<td>0.236</td>
<td>0.217</td>
<td>0.180</td>
<td>0.172</td>
<td>0.145</td>
<td>0.121</td>
<td></td>
<td></td>
<td></td>
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</table>

* The maximum values of Schmid factor for each grain boundary are shaded.

Fig. 5.1 shows the stress-strain curves of the Cu bicrystal models with <0 0 1> tilt axes and various misorientation angles under tensile loading with free boundary conditions along the X and Z directions. The curves are divided into two groups. Figs. 5.1(a) and 5.1(b) are for GBs with θ ≤ 43.60° and GBs with θ ≥ 47.93°, respectively. It was found that the maximum tensile stress was associated with the nucleation of partial dislocations, agreeing well with previous research studies [30, 41, 84]. At the elastic loading stage, the stress-strain curves overlap. This indicates that the Young modules are quite similar. The maximum tensile stress changes considerably with increasing misorientation angles.
Fig. 5.1 Stress-strain curves of Cu bicrystal models with $<0\overline{0}1>$ tilt axes and various misorientation angles under tension loading with free boundary conditions along the X and Z directions.

(a) misorientation angles from 18.93° to 43.60°; (b) misorientation angles from 47.93° to 71.08°.

The maximum tensile stress collected from Fig. 5.1 is plotted as a function of the GB misorientation angle in Fig. 5.2(a). It can be seen that the maximum tensile stress decreases gradually as the misorientation angle increases. In order to analyse the dependency of the maximum tensile stress on lattice orientation, simulations using single crystals with the same crystallographic orientations as the upper grain were also performed. The results are included in Fig. 5.2(a) for comparison purposes. The curves of the bicrystal and single crystal models show very similar trends. However, the single crystal models have higher values than the bicrystal models. This indicates that the GB assists dislocation nucleation.

5.3.2 Mechanisms of dislocation nucleation from GBs with [001] tilt axes

The Schmid factors for partial dislocations in the simulation models are given in Table 5.1. The maximum resolved shear stress is estimated by dividing the maximum tensile stress by the Schmid factor. Fig. 5.2 (b) shows maximum resolved shear stress as a function of the misorientation angle. Similar to the maximum tensile stress, the maximum resolved shear stress decreases gradually...
for both single crystals and bicrystals as the misorientation angle increases. This indicates that the dependence of tensile stress on the misorientation angle is a non-Schmid behaviour. It was stated by Nagata and Yoshida [85] that the maximum resolved shear stress in Cu is insensitive to the lattice orientation under tensile deformation, exactly explaining the Schmid behaviour. However, Ogata et al. [86] found that the impact of non-glide stress components on the slip plane on the maximum resolved shear stress was considerable. Steinmann et al. [87] went further and demonstrated that the yield stress required for dislocation nucleation decreased in the presence of tensile stress perpendicular to the slip plane. In the models studied in this section, the magnitude of the non-glide stress (tensile stress perpendicular to slip planes) rises with increasing lattice orientation around the [0 0 1] axis. This increase in non-glide stress is responsible for a decrease in the maximum resolved shear stress.

Fig. 5.2 (a) Maximum tensile stress and (b) maximum resolved shear stress versus misorientation angle for Cu bicrystal models under tensile deformation with free boundary conditions along the X and Z directions.

Fig. 5.3 shows dislocation activities and atomistic configurations for $\Sigma$17 (4 1 0) GB at 1 K during tensile deformation. Visual inspection of the results of the MD simulations revealed that the maximum tensile stress corresponds to the nucleation of partial dislocations. The atoms in the system are coloured according
to the CNA parameter, which is a scalar quantity. The colouration is designed to indicate defects, including dislocations, stacking faults and interfaces. The red atoms show the location of the stacking fault, and the blue atoms form the GB planes and dislocation cores. Atoms with perfect structure have been removed to facilitate viewing of the defective configurations. Prior to the maximum tensile stress point, the GB region becomes thicker, as evidenced by an increase in the thickness of the area identified as the boundary plane by CNA in the elastic stage. Also, the kite-shaped E SUs are severely distorted when accommodating the imposed tensile strain during the coarsening process. In Fig. 5.3 (b), the onset of plasticity is activated by an array of nucleation of the partial dislocation loops with edges and screw characters from its interface plane into the upper grain and lower grain simultaneously. The DXA analysis, as shown in Fig. 5.3, indicates that the dislocation slip occurs on both the $(1 1 1)$ and $(1 1 \bar{1})$ planes in the upper grain, and on the $(\bar{1} 1 1)$ and $(1 \bar{1} 1)$ planes in the lower grain. This leads to four nucleated partial dislocations $(1/6[\bar{1} \bar{1} 2])$ and $1/6[1 1 2]$ in the upper grain and $1/6[1 \bar{1} 2]$ and $1/6[\bar{1} 1 2]$ in the lower grain) linked back to the boundary plane by a series of intrinsic stacking faults. The activation of two slip systems from the interface is consistent with Schmid factor analysis, suggesting that both slip systems have the maximum Schmid factor (see in Table 5.1).
Fig. 5.3. Dislocation activities and atomistic configurations for $\Sigma 17 (4 1 0)$ GB at 1 K during free tensile deformation process. All images are coloured by CNA. Atoms with a perfect FCC structure are blue, the red atoms organise the TGB plane and the dislocation core, and the continuous light blue atoms represent the stacking fault.

Fig. 5.4 shows the dislocation activities and atomistic configurations for $\Sigma 17 (5 3 0)$ GB at 1 K during tensile deformation. The atoms are coloured according to their CNA values. It can be seen that the dislocation nucleates from the $\Sigma 17 (5 3 0)$ GB are the same as for the $\Sigma 17 (4 1 0)$ GB, though the corresponding misorientation angles are different. Generally, the activated slip systems in the bicrystal models studied in this thesis are identical under free boundary conditions.
Fig. 5.4. Dislocation activities and atomistic configurations for $\Sigma 17$ (530) GB at 1 K during tensile deformation process. Atoms with perfect FCC structures have been removed and atoms of different colours represent the same areas described in Fig. 5.3.

Fig. 5.5 shows the stress-strain curves of Cu bicrystals subjected to tensile deformation under constrained boundary conditions along the X and Z directions. Figs. 5.5(a) and 5.5(b) depict the results for $\theta \leq 43.60^\circ$ and $\theta \geq 47.93^\circ$, respectively. The maximum tensile stress under constrained boundary conditions is dramatically higher than under free boundary conditions. This is attributable to the stress developed in the transverse direction (X and Z directions) under tensile loading.
Fig. 5.5 Stress-strain curves of Cu bicrystal models with the <0 0 1> tilt axes and various misorientation angles under tension loading under constrained boundary conditions along X and Z directions.

(a) misorientation angles from 18.93° to 43.60°; (b) misorientation angles from 47.93° to 71.08°.

Fig. 5.6 shows dislocation activities and atomistic configurations for \( \Sigma 5 \ (2 \ 1 \ 0) \) GB at 1 K during tensile deformation. All of the atoms are coloured according to their CNA values. The red atoms show the stacking fault, and the blue atoms indicate the GB planes and dislocation cores. The atoms with perfect structure have been removed in order to facilitate the viewing of the defect configurations. It can be seen that the dislocation slip occurs on both the \( [1 1 1] \) and \( [1 
\bar{1} \ 1] \) planes in the upper grain, and on the \( [\bar{1} \ 1 \ 1] \) and \( [1 \ 1 \bar{1}] \) planes in the lower grain. This leads to four nucleated partial dislocations \( \{1/6[\bar{1} 
\bar{1} \ 2] \) and \( 1/6[1 \ 1 \ 2] \) in the upper grain and \( 1/6[1 \ \bar{1} \ 2] \) and \( 1/6[ \bar{1} \ 1 \ 2] \) in the lower grain) linked back to the boundary plane by a series of intrinsic stacking faults. Obviously, unlike the free boundary conditions, the constrained boundary conditions do not change plastic deformation behaviour since the dislocation nucleates and the slip are on the same slip planes for the two boundary conditions. After the dislocation nucleates and emits from the GB plane, some voids appear, as shown in Fig. 5.6 (b). The further increased tensile strain results in the formation of voids and coalescence until the GB is absolutely separated (ultimate fracture). This is different to the
failure mode which occurs under free boundary conditions. Under free boundary conditions, the failure of GBs is related to dislocation activities (dislocation nucleation and glide). This difference is probably because the multiaxial stress state caused by the constrained boundary conditions makes the failure mode more brittle than that under free boundary conditions.

![Dislocation activities and atomistic configurations](image)

(a) $\varepsilon = 0\%$
(b) $\varepsilon = 10.6\%$
(c) $\varepsilon = 10.8\%

Fig. 5.6. Dislocation activities and atomistic configurations for $\Sigma 5 \{2 \ 1 \ 0\}$ GB at 1 K during tensile deformation. Atoms with perfect FCC structures have been removed and atoms of different colours represent the same areas described in Fig. 5.3.

The maximum tensile stress and the maximum resolved shear stress are plotted as functions of the GB misorientation angles in Fig. 5.7. The results for single crystals with the same crystallographic orientation as the upper grain are also shown in this figure. For single crystals, the maximum tensile stress is reduced gradually with an increasing rotation angle around the [0 0 1] axis, similar to the cases under free boundary conditions. However, the maximum tensile stress for the bicrystal models varies greatly. There are two local maximum points for the bicrystal models, as shown in Fig. 5.7 (a), corresponding to two low $\Sigma$GBs ($\Sigma 13$ and $\Sigma 5$). This suggests that the lateral confinement of the GBs affects the tensile strength of the low $\Sigma$GBs.
Fig. 5.7 (b) shows maximum resolved shear stress versus misorientation angle under constrained boundary conditions. Compared with the cases under free boundary conditions, the maximum resolved shear stresses for the constrained boundary conditions are reduced. This is mainly attributed to the increased non-gliding stress (tensile stress perpendicular to slip planes). Further, for both single crystals and bicrystals, the trend in changes to curves (non-Schmid behaviour) is not obvious, unlike the free boundary condition cases. One can notice that there is an abrupt drop at the orientation angle of \( \theta = 56.15 \). A visual inspection indicates that this is due to a change in dislocation activities. Although the slip systems remain unchanged, the partial dislocations nucleate from the \( 1/6[2 \overline{1} 1] \) to \( 1/6[1 1 2] \) when the misorientation angle increases beyond \( 53.13^\circ \). As shown in Table 5.1, the maximum Schmid factor (shaded values) occurs along the \( 1/6[2 \overline{1} 1] \) direction when \( \theta < 53.13^\circ \), while it changes to the \( 1/6[1 1 2] \) direction when \( \theta \geq 53.13^\circ \).

![Graphs showing maximum tensile stress and maximum resolved shear stress versus misorientation angle](image)

Fig. 5.7 (a) Maximum tensile stress and (b) maximum resolved shear stress versus the misorientation angle in Cu bicrystals under tensile deformation with constrained boundary conditions.
5.4 Tensile deformation response of bicrystal models with $[1 \bar{1} 0]$ tilt axes

5.4.1 Analysis of the stress-strain of GBs with $[1 \bar{1} 0]$ tilt axes

Fig. 5.8 shows the tensile stress-strain curves of the Cu bicrystal model with a $[1 \bar{1} 0]$ tilt axis and various misorientation angles under free boundary conditions. The curves are divided into two groups: one with $\theta \leq 109.47^\circ$ is shown in Fig. 5.8(a) and the other group with $\theta \geq 111.53^\circ$ is shown in Fig. 5.8(b). Similar to the cases studied in Section 5.2.1, maximum tensile stress is accompanied by the nucleation of the partial dislocations. It is well known that GBs or free surfaces mainly provide dislocation nucleation sites in polycrystalline materials during the plastic deformation process. In the present study, there was one exceptional case involving the $\Sigma 3$ $(1 1 1)$ coherent twin boundary: the dislocations nucleate from the grain interior rather than from the GB boundary. It can be seen in Fig. 5.8 (b) that the case with the $\Sigma 3$ $(1 1 1)$ coherent twin boundary has the highest tensile strength, which is likely due to its simple interface structures and because it has the lowest GB energy.

Fig. 5.9 compares the maximum tensile stresses of bicrystals and single crystals with the same crystallographic orientations as the upper grain of the bicrystals under free boundary conditions. It can be seen that the maximum stress of the single crystal gradually increases with the misorientation angle and then gradually decreases when the misorientation angle goes beyond $109.5^\circ$. For the bicrystals, the tensile response follows the same trend as the single crystal cases when $\theta \leq 109.5^\circ$. A sudden drop is observed at $\theta = 109.5^\circ$, and then the maximum tensile stress increases with the misorientation angle again. The stress drop is associated
with the character of the boundary structures. GBs with misorientation angles of less than 109.5° are composed of D SUs. All the GBs with of misorientation angles of larger than 109.5° are composed of E SUs. Sansoz and Molinari [40] reported that the intrinsic free volume of the E structure unit can change the shear deformation mode.

![Fig. 5.8 Stress-strain curves of Cu bicrystal models with <110> tilt axes and various misorientation angles under tension loading with free boundary conditions along X and Z directions.](image)

(a) misorientation angles from 26.53° to 109.47°; (b) misorientation angles from 114.53° to 166.56°.

![Fig. 5.9 (a) Maximum tensile stress and (b) maximum resolved shear stress versus misorientation angle in Cu bicrystals with <110> tilt axes under tensile deformation with free boundary conditions.](image)
5.4.2 Mechanisms of dislocation nucleation from GBs with [1 1 0] tilt axes

Fig. 5.10 shows snapshots of three GBs with \( \theta \leq 109.5^\circ \) at the beginning of plastic deformation. For the \( \Sigma 19 \) (1 1 6) GB with an orientation angle of 26.5\(^\circ\), when the stress reaches its peak value, a series of Shockley partial dislocations nucleate from the GB and glide onto the (1 1 1) and (1 1 1) planes, which are the secondary and primary slip planes. These two partial dislocations meet and intersect to form a 1/6[1 0 1] stair-rod dislocation.

As identified in Fig. 4.9 (d)-(g), the GBs with the misorientation angles of 50.5\(^\circ\) < \( \theta \) < 109.5\(^\circ\) have the dissociated structures. Taking the \( \Sigma 33 \) (2 2 5) GB as an example, it is found that the intrinsic stacking faults (ISF) extend from one side of the GB due to asymmetric dislocation dissociation. With an increase of the imposed tensile strain, the length of ISF facets is reduced. When the yield point is reached, dislocation nucleation occurs where the ISF facets and the GB intersect, as shown in Fig. 4.9 (j).

The nucleated 1/6[1 1 2] partial dislocation glides on the (1 1 1) plane, generating an extrinsic stacking fault behind, as shown in Fig. 5.12 (d). The Schmid factor analysis reveals that the slip plane is a secondary slip plane, indicating that the presence of ISF facets promotes dislocation activity on secondary slip planes.

In the case of the higher misorientation angle (\( \Sigma 17 \) (2 2 3)), two Shockley partial dislocations with Burgers vectors of 1/6[1 2 1] and 1/6[2 1 1] are only nucleated from the primary slip system. Spearot et al. [89] pointed out that the spacing between the ISF facets was critical for the failure mode of the GB. It can be seen from the simulation results that the spacing between the ISF facets is reduced with increasing misorientation angles of 50.48\(^\circ\) < \( \theta \) < 109.47\(^\circ\), leading to a change from dislocation nucleation from the secondary slip system to dislocation...
nucleation from both primary and secondary slip systems, and eventually to dislocation nucleation from the primary slip system.

Fig. 5.10. Dislocation activities and atomistic configurations for (a) $\Sigma 19 (1 1 6)$ GB, (b) $\Sigma 33 (2 2 5)$ GB and (c)-(d) $\Sigma 17 (2 2 3)$ GB during tensile deformation with free boundary conditions.

Fig. 5.11 shows dislocation activities and atomistic configurations for bicrystals with $\Sigma 9 (1 1 4)$ and $\Sigma 11 (1 1 3)$ GBs. It has been shown in Section 4.3.2 that the $\Sigma 9 (1 1 4)$ GB consists of C and D SUs, while the $\Sigma 11 (1 1 3)$ GB is entirely composed of C SUs, resulting in a lower boundary energy. In Figs. 5.11 (a) and (b), the Shockley partial dislocations nucleate from the $\Sigma 9 (1 1 4)$ GB into two grains – an upper grain and a lower grain. The DXA analysis suggests that two partial dislocations with the Burgers vectors of $1/6[1 1 \bar{2}]$ and $1/6[1 1 2]$ nucleate from the GB and glide on the $(1 1 1)$ and $(1 1 \bar{1})$ planes, which are both primary slip
planes which both have a Schmid factor of \( SF_{(111)}^{max} = SF_{(11\bar{1})}^{max} = 0.471 \). A set of extrinsic stacking faults connecting the partial dislocation core back to the GB can be observed. The extrinsic partial dislocations are induced by the evolution of the C SUs.

The atomistic configurations of the \( \Sigma 11 \ (1 \ 1 \ 3) \) GB are shown in Figs. 5.11 (c) and (d). For this GB, when the maximum stress is reached at \( \varepsilon = 9.98\% \), dislocation nucleation occurs on the (1 1 1) and (1 1 \( \bar{1} \)) planes, which are both primary slip planes with the same Schmid factor of \( SF_{(111)}^{max} = SF_{(11\bar{1})}^{max} = 0.471 \). Two nucleated partial dislocations glide on their own planes in the upper grain and lower grain. At \( \varepsilon = 10.02\% \), the lattice dislocation loops with a V-shape are triggered and slip on the (1 \( \bar{1} \) 1) and (\( \bar{1} \) 1 1) planes. Due to the stable boundary structure of the \( \Sigma 11 \ (1 \ 1 \ 3) \) GB with relatively low GB energy, it is difficult for the V-shaped dislocation loops to nucleate directly from the GB. Instead, these partial dislocations nucleate from the grain interior. Aside from the extrinsic stacking fault, a twin fault is also observed at the GB during tensile deformation, as shown in Fig. 5.11 (c). The evolution of the C SUs leading to the extrinsic stacking fault and twin fault are interpreted in Figs. 5.11 (e)-(f).

A detailed inspection of the snapshots shown in Figs. 5.11 (e)-(f) indicates that free boundary conditions cause a series of C SUs to shrink, and this leads to dislocation nucleation. Specifically, as shown in Fig. 11 (e), Atom 1 translates along the negative X direction as the first C unit shrinks, which causes the atoms residing on plane ‘a’ to slip towards the GB, and the atoms on plane ‘b’ to slip out of the GB. As a result of this relative shift of the slip systems, the first partial dislocation nucleation with the ISF occurs. Following the same process, the translation of Atom 2 leads to the second partial dislocation nucleation through a
relative shift of the atoms on plane ‘b’ and plane ‘c’. It is worth noting that the slip
direction caused by Atom 2 on plane ‘b’ is opposite to the direction caused by
Atom 1, which drives the atoms on plane ‘b’ to turn back to the perfect FCC
position and form an extrinsic stacking fault, as shown in Fig. 5.11 (e)-(f).

![Diagrams showing dislocation activities and atomistic configurations](image)

Fig. 5.11 Dislocation activities and atomistic configurations for (a)-(b) $\Sigma 9 (1 1 4)$ and (c)-(d) $\Sigma 11 (1 1 3)$ GBs
during tensile deformation; (e)-(f) a detailed inspection of the snapshots of the evolution of C SU.

The nucleation mechanism of the extrinsic stacking fault on the GB via two partial
dislocations emitted in neighbouring compact planes is observed in the case of
the $\Sigma 9 (1 1 4)$ GB. However, unlike to the case of the $\Sigma 9 (1 1 4)$ GB, the
consecutive shrinkage of the C SUs along the GB provides sources of continuous nucleation for the consequent partial dislocations, resulting in the broadening of the twinning regions. As shown in Figs. 5.11 (f) and (g), the translations of Atom 3 and Atom 4 along the negative X-direction result in the broadening of the twin boundary to four and five (1 1 1) lattice spacing.

For the $\Sigma 3$ (1 1 1) GB, the maximum tensile stress demanded for the dislocation nucleation is the same as that of the corresponding single crystal (see 5.9 (a)), which reveals that the GB isn’t the source for dislocation nucleation. This kind of boundary has simple boundary structures with the lowest GB energy of all investigated cases. Free boundary conditions provide no free volume for atoms to move or rearrange themselves when the bicrystal model is subjected to tensile deformation. It is difficult, therefore, for partial dislocations to nucleate or emit from the GB. To accommodate higher tensile strain, the dislocation nucleation occurs in the grain interior, as shown in Fig. 5.12 (a). The same phenomenon can be observed in the single crystals. It can be seen that dislocation slip occurs on three \{1 1 1\} planes, leading to three sets of dislocation loops with edge and screw characters. According to the analysis of the Schmid factor, all of them are favourable slip planes with a maximum Schmid factor of $SF_{(1\bar{1}1)}^{max} = SF_{(1\bar{1}1)}^{max} = SF_{(11\bar{1})}^{max} = 0.314$.

The $\Sigma 171$ (11 11 10) GB is considered to be a vicinal twin boundary due to small deviations in the lattice orientation relative to the coherent twin boundary. As shown in Fig. 5.12 (b), the GB is stepped and has also dissociated by emitting intrinsic stacking faults into grains. The defects related to the steps have been confirmed to be $\frac{1}{3} < 1 1 1 >$ GB disconnections. Analogous to the Frank partial
dislocation, these disconnections possess a Burgers vector of $\frac{1}{3} < 1 1 1 >$ oriented perpendicularly to the twin boundary plane. Marquis and Medlin [88] reported that $\frac{1}{3} < 1 1 1 >$ disconnections can relax into a compact core structure or a dissociated Shockley partial dislocation, referred to as ‘interior’ and ‘exterior’ disconnections, respectively. The $\Sigma 171$ (11 11 10) GB has alternating ‘exterior’ disconnections, which dissociate by emitting Shockley partial dislocations into the lattice, with a stair-rod dislocation left behind ($\frac{1}{3} < 1 1 1 > \rightarrow \frac{1}{6} < 1 1 2 > + \frac{1}{6} < 1 1 0 >$). It needs to be mentioned that the onset of plasticity is triggered at a very low tensile strain ($\varepsilon = 1.02\%$), compared to the other cases. The Shockley partial dislocations have already nucleated from the GB plane in the ground state, thus a low stress is required to drive them to emit.

Fig. 5.12. Dislocation activities and atomistic configurations for (a) $\Sigma 3$ (1 1 1) GB and (b)-(c) $\Sigma 171$ (11 11 10) GBs during tensile deformation.
Fig. 5.13 shows dislocation nucleation from the $\Sigma 11$ (3 3 2) GB in Cu bicrystals. As stated in Section 4.3.2, all GBs with misorientation angles greater than 109.5° are composed of E SUs. The circled regions in Figs. 5.13 (d) and (e) show the magnified views of the corresponding interface structures of Fig. 5.13 (a) and (c). It can be seen from Fig. 5.13 (a) and (d) that the $\Sigma 11$ (3 3 2) GB consists of both E and D SUs. During tensile loading under free boundary conditions, a series of very short ISF facets is first nucleated from the GB plane, as shown in Fig. 5.13 (b). These ISF facets are identified as Shockley partial dislocations slipping on the primary planes. The DXA analysis indicates that two partial dislocations with Burgers vectors of 1/6[1 1 $\overline{2}$] and 1/6[1 1 2] nucleate from the GB and glide on the (1 1 1) and (1 1 $\overline{1}$) planes in the upper and lower grains, respectively. Both these planes are primary slip planes with the Schmid factor of $SF_{(111)}^{max} = SF_{(111)}^{max} = 0.429$. Some nucleated partial dislocations then propagate away from the GB, causing the ISF facets to become shorter, or even to be absorbed by the GB.

The evolution of the E SUs during the dislocation process is given in Figs. 5.13 (d) and (e). Prior to the dislocation nucleation, all E SUs are connected by the D units. The E SU located on the left is tilted downward and is marked by Atom a–Atom f, while the right one tilted upward is indexed by Atom g–Atom l. As the maximum stress is reached, the partial dislocation emits from the downward E SU into the upper grain, facilitated by a relative shift of the opposing (1 1 1) slip plane. In other words, Atom d slips out of the E SU while Atom e slips into the E SU along the (1 1 1) plane. Following the same process, Atoms k and l slip on the opposing (1 1 $\overline{1}$) plane, leading to dislocation nucleation from the upward E SU into the lower grain. The relative motion of Atoms d, e, k and l reduces and collapses the
free volume of the E SUs positioned at the end of the {111} plane, and eventually evolves the E SUs into the C SUs. The snapshots of the dislocation nucleation for all other GBs with $\theta > 109.5^\circ$ are given in Fig. 5.14. Consistent with the previous cases, the E SUs directly serve as the sources of the dislocation nucleation. The Shockley partial dislocations are triggered and glide on the (111) and (1 1 1) planes in the upper and lower grains respectively. Both of these planes are the primary slip planes with the Schmid factor of $SF_{(111)}^{\text{max}} = SF_{(111)}^{\text{max}} = 0.429$. Although all dislocation nucleation events are caused by the evolution of E SUs into C SUs, the specific atomic movement corresponding to this evolution is different from case to case. In the case of the $\Sigma 9$ (2 2 1) GB, the E SUs come in pairs (referred to as left-hand and right-hand). For example, the left and right E SUs share two common atoms, indexed Atoms e and f in the left E SU, and Atoms g and i in the right E SU unit, as shown in Fig. 5.13 (d). The movement of Atoms e and f relative to each other on the (1 1 1) plane and of Atoms g and i on the (1 1 1) plane collapses the E SUs and changes them into C SUs. For the $\Sigma 73$ (6 6 1) GB, all E SUs are almost symmetric along the X direction, unlike other cases where the E tilts upward or downward. Atom e first translates along the positive X direction, attempting to reduce the pocket of free volume of the E SU. At the same time, Atoms d and f are driven by the increased interatomic force due to the movement of Atoms e and k to slip out of the E SU. This slip of Atoms d and e on the (1 1 1) plane and of Atoms e and f on the (1 1 1) plane facilitates the dislocation nucleation from the GB.
Fig. 5.13. Dislocation activities and atomistic configurations for $\Sigma 11$ (3 3 2) GB at 1 K during the tensile deformation process. Atoms with perfect FCC structures have been removed and atoms of different colours represent the same areas described in Fig. 5.3.
Fig. 5.14. Dislocation activities and atomistic configurations for (a) $\Sigma 9 (2 \ 2 \ 1) \ GB$, (b) $\Sigma 19 (3 \ 3 \ 1) \ GB$, (c) $\Sigma 73 (6 \ 6 \ 1) \ GB$ during tensile deformation.
The tensile responses for the Cu bicrystal models with [1 1 0] tilt axes and different misorientation angles under constrained boundary conditions are similar to those for the [0 0 1] Cu bicrystal models. The maximum stress for each case is considerably larger than that for the corresponding case with free boundary conditions.

Fig. 5.15. Dislocation activities and atomistic configurations for $\Sigma 9$ (2 2 1) GB during constrained tensile deformation.

Fig. 5.15 shows dislocation activities for the $\Sigma 9$ (2 2 1) GB under constrained boundary conditions. The dislocation nucleation from the GB is the same as that under free boundary conditions. The dislocation nucleation is generated from the E SUs directly and facilitated through the collapse of the pocket of free volume (E SUs). The only difference is that under constrained boundary conditions the uniformity and length of the ISF facets that nucleate prior to the dislocation propagation. Fig. 5.1b (b) suggests that the ISF facets nucleate less frequently and the length of ISF is shorter than its length under free boundary conditions. This
implies that the stresses parallel to the GB may restrain the collapse of the free volume of E SUs and further suppress the dislocation nucleation.

5.5 Summary

MD simulations were conducted to investigate the dislocation nucleation behaviour of tilt GBs in Cu bicrystals with misorientation axes of \(<0 0 1>\) and \(<1 1 0>\). Both ‘free’ and ‘constrained’ boundary conditions were applied in the simulations. The simulation results revealed that the stress state played a significant role in the deformation mechanism. The relationships between boundary strength (maximum tensile stress and maximum resolved shear stress) and boundary structure were quantified. The atomistic mechanisms of dislocation nucleation in various GBs were illustrated in detail. This thesis establishes a relationship for the dislocation nucleation threshold, on a statistical basis. Furthermore, a post-yield analysis was performed to demonstrate correlations with the dislocation length. This chapter shows that: (1) a discontinuity in the periodic local stress distribution in the GB interface provides a useful indicator for the post-yield dislocation response; (2) the process of dislocation nucleation under compression involves the collapse of accumulations of free volume at the grain boundaries; (3) the Schmid factor analysis described by Spearot [44,45] is effective for predicting the slip system for the first dislocation nucleation in bicrystal simulations.

In this fundamental simulation case examined in this thesis, with high strain rates and 100% metal purity, the overall accuracy of the correlations is not as important as the implications of the statistical significance of the factors. The findings indicate that the apparently random process of dislocation nucleation can be
attributed to real, measurable physical features of materials’ micro-structures. With more detailed simulations in the future, it may be possible to predict nucleation thresholds in complex metal alloys with more realistic strain rates.
Chapter 6

Conclusions and recommendations

This thesis focused on understanding the role of grain boundary and dislocation nucleation in FCC materials. Molecular dynamics simulations were conducted throughout the work. This is an important subject given the interest in various tilt axes and misorientation angles. The two main parts of this thesis are: (1) the simulation of grain boundaries with different tilt axes and misorientation angles, and then the calculation of minimal grain boundary energies; and (2) the simulation of tensile deformation responses in bicrystal models under both free and constrained boundary conditions, with rotation axes of [001] and [110]. The significant contributions of this work are summarised in the following sections.

6.1 Analysis of GB structures and local minimal GB energies

In this thesis, the main research methods were MS and MD simulations. The MS simulations were conducted to study the GB structures and GB energies of 1184 GBs of Cu and Al with 66 different tilt axes and a wide range of misorientation angles. The MD simulations were applied to analyse the procedures of dislocation nucleation and tensile deformation of GBs with tilt axes of [001] and [110]. The study shows that:

1. Local minimal GB energies corresponded to certain GB structures. For instance, \( \Sigma 11 \ (1\ 1\ 3) \) and \( \Sigma 3 \ (1\ 1\ 1) \) GBs, which were composed entirely of C and D SUs respectively. Also, the \( \Sigma 9 \ (2\ 2\ 1) \) GB consisted entirely of E SUs.
2. Tilt axis affects GB structures. For the tilt axis [0 0 1], all the tilt GBs were composed of topologically identical E SUs, which differed only in the distances between adjacent SUs. For the tilt axis [1 1 0], all GBs except $\Sigma_{11}$, $\Sigma_3$ and $\Sigma_{9}$ consisted of a combination of C, D and E SUs.

3. In Chapter 4, the two FCC metals, Cu and Al, were found to have similar GB structures in the MS simulations. After the process of energy minimisation, their GB structures with local minimal GB energies were found to be composed of the same types of SUs. The simulation results from this study give us a better understanding of the GBs of FCC materials.

6.2 Deformation mechanisms of GBs in Cu bicrystal

The MD simulations of Cu single crystals and bicrystals with [0 0 1] and [1 1 0] tilt GBs under uniaxial loading were performed to investigate the mechanism of dislocation nucleation from the GBs. Both free and constrained boundary conditions were applied in the simulations.

It was found from the MD simulations with the [0 0 1] tilt axis that:

1. Under free boundary conditions, the maximum resolved shear stress gradually decreased for both single crystals and bicrystals in response to increases of the misorientation angle. Non-Schmid behaviour was observed.

2. Under constrained boundary conditions, the maximum tensile stress was dramatically higher than it was under free boundary conditions, which was attributable to the stress developed in the transverse direction during uniaxial loading.
3. For all cases, two slip systems with the maximum Schmid factor were activated at the maximum tensile stress, leading to four partial dislocations linked back to the GB plane by a series of intrinsic stacking faults. It was found from the MD simulations with [1 1 0] tilt axes that:

1. Maximum tensile stress gradually increased with the misorientation angle, and then decreased after the misorientation angle went beyond 109.5°.

2. For misorientation angles within the range of 50.5°<θ<109.5°, intrinsic stacking faults extended from one side of the boundary plane due to asymmetric dislocation dissociation. When the maximum tensile stress was reached, dislocation nucleation occurred while the ISF facets and the boundary plane intersected. In response to increases in the misorientation angle within this range, the deformation mode changed from dislocation nucleation from the secondary slip system to a mixture of dislocation nucleations from both primary and secondary slip systems, and eventually to dislocation nucleation that was exclusively from the primary slip system.

3. At the misorientation angle of θ=109.5°, the GB structure was simple and the GB energy was at its lowest. As a result there was no partial dislocation nucleated from the GB when the tensile stress reached its maximum value.

4. For misorientation angles θ>109.5°, the intrinsic GB structure became the predominant factor in the deformation mechanisms of the GBs. The dislocation nucleation was realised by the transformation of the E SUs of the boundary planes.
6.3 Recommendations for future work

1. Nucleation mechanisms of asymmetric GBs: In Chapter 6, tensile deformations on the symmetric tilt GBs with [0 0 1] and [1 $\bar{1}$ 0 ] tilt axes were simulated. However, the experimental characterisation shows that most boundaries in polycrystalline materials are actually asymmetric tilt GBs [88, 89]. Asymmetric tilt GBs present an interesting case for studying dislocation nucleation behaviours in the future.

2. Other types of material systems: In this thesis GB structures, energies and deformation mechanisms in the FCC materials, Cu and Al, were investigated by way of MC and MD simulations. Similar simulations could be applied to BCC and HCP materials.

3. Combination of MD simulations with experimental observations: In thesis, the main focus was on the theoretical field of applying MD simulations to analyse the tensile deformation of bicrystal FCC materials. In the next step, the results of the simulations will be compared with experimental observations to get a better understanding of dislocation nucleation phenomena.

4. More variables should be considered in future work. For example, this thesis sets 1 K as temperature parameter throughout the simulation process. In the next step, not only temperatures but also various strain rates will be variables in MD simulations. In addition, the results of simulations will be compared with experimental observations.
References


N. Nagata, S. Yoshida, Deformation of copper single crystals and polycrystals at high strain rates, Japan Institute of Metals, 1972.


Affiliation I: Program of lattice orientation

clear;
A=[x1 y1 z1; x2 y2 z2; x3 y3 z3];
A(1,:) = A(1,:)/norm(A(1,:));
A(2,:) = A(2,:)/norm(A(2,:));
A(3,:) = A(3,:)/norm(A(3,:));

theta=90;
theta=theta*pi/180;
R=[cos(theta), -sin(theta), 0; sin(theta), cos(theta), 0; 0, 0, 1]
B=R*A;

%check
acos(dot(A(1,:),B(1,:)))*180/pi

Affiliations II: Program of tensile deformation

clear
units metal
dimension 3
boundary p p p
atom_style atomic
variable lattice equal 3.615
variable cna equal "v_lattice*(1+1/sqrt(2))/2"
read_data 210.dat
replicate 2 1 40

# -------- Define Interatomic Potential --------------
pair_style eam/alloy
pair_coeff * * Cu_mishin1.eam.alloy Cu Cu Cu Cu Cu
neighbour 2.0 bin
neigh_modify delay 1 check yes

# -------- Define Settings -------------------------
compute cna all cna/atom ${cna}
compute eng all pe/atom
compute eatoms all reduce sum c_eng

# -------- EQUILIBRATION ---------
reset_timestep 0
timestep 0.001
velocity all create 1 12345 mom yes rot no
fix 1 all npt temp 1 1 1 iso 0 0 1 drag 1

# Set thermo output
thermo 1000
thermo_style custom step pe lx ly lz press pxx pyy pzz temp

# Run for at least 10 picosecond (assuming 1 fs timestep)
run 20000
unfix 1

# Store final cell length for strain calculations
variable tmp equal "ly"
variable L0 equal \${tmp}
print "Initial Length, L0: \${L0}"

######################################
# DEFORMATION
reset_timestep 0
fix 1 all npt temp 1 1 1 x 0 0 1 z 0 0 1 drag 1
variable srate equal 1.0e9
variable srate1 equal "v_srate / 1.0e12"
fix 2 all deform 1 y erate \${srate1} units box remap x

# Output strain and stress info to file
# for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]
# p2 is in GPa
variable strain equal "(ly - v_L0)/v_L0"
variable p1 equal "v_strain"
variable p2 equal "-pxx/10000"
variable p3 equal "-pyy/10000"
variable p4 equal "-pzz/10000"
fix def1 all print 1000 "$\{p1\} \{p2\} \{p3\} \{p4\}" file Cu_sig_t.def1.txt screen no

# Use cfg for AtomEye
dump 1 all cfg 1000 dump.tensile_*.cfg mass type xs ys zs c_cna fx fy fz
dump_modify 1 element Cu Cu Cu Cu Cu

# Display thermo
thermo 1000
thermo_style custom step v_strain temp v_p2 v_p3 v_p4 ke pe press
run 200000

# SIMULATION DONE
print "All done"

Affiliations III: Program of energy minimization
# -------- Define Settings ---------------------
compute csym all centro/atom \${lattype}
compute eng all pe/atom
compute eatoms all reduce sum c_eng

# -------- Run Minimization ---------------------
reset_timestep 0
thermo 10
thermo_style custom step pe lx ly lz press pxx pyy pzz c_eatoms
min_style cg
minimize \${etol} \${ftol} \${maxiter} \${maxeval}

# -------- Run Minimization 2 ---------------------
# Now allow the box to expand/contract perpendicular to the grain boundary
reset_timestep 0
thermo 10
thermo_style custom step pe lx ly lz press pxx pyy pzz c_eatoms
fix 1 all box/relax y 0.0 vmax 0.01
min_style cg
minimize \${etol} \${ftol} \${maxiter} \${maxeval}

# -------- Calculate GB Energy ---------------------
variable esum equal "v_minimumenergy * count(all)"
variable xseng equal "c_eatoms - (v_minimumenergy * count(all))"
variable gbarea equal "lx * lz * 2"
variable gbe equal "(c_eatoms - (v_minimumenergy * count(all)))/v_gbarea"
variable gbemJm2 equal ${gbe}*16021.7733
variable gbernd equal round(${gbemJm2})
print "After third minimization:"
print "GB energy is ${gbemJm2} mJ/m^2"

# Store number of atoms for overlap criterion, i.e., do not rerun equivalent configurations
variable atomprev equal ${natoms}