Influences of Stress-Driven Grain Boundary Motion on Microstructural Evolution in Nanocrystalline Metals

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Abstract

Nanocrystalline (NC) metals with averaged grain size smaller than 100 nm have shown promising mechanical properties such as higher hardness and toughness than conventional coarse-grained metals. Unlike conventional metals in which the deformation is controlled by dislocation activities, the microstructural evolution in NC metals is mainly dominated by grain rotation and stress-driven grain boundary motion (SDGBM) due to the high density of grain boundaries (GBs). SDGBM is thus among the most studied modes of microstructural evolution in NC materials with particular interests on their fundamental atomistic mechanisms.

In the first part of this thesis, molecular dynamics simulations were used to investigate the influences of Triple Junctions (TJs) on SDGBM of symmetric tilt GBs in copper by considering a honeycomb NC model. TJs exhibited asymmetric pinning effects to the GB migration and the constraints by the TJs and neighboring grains led to remarkable non-linear GB motion in directions both parallel and normal to the applied shear. Based on these findings, a generalized model for SDGBM in NC Cu was proposed.

In the second part, the interaction of SDGBM with crack, voids and precipitates was investigated. It was found that depending on the GB structure, material type and temperature, there is a competition between different atomistic mechanisms such as crack healing, recrystallization and GB decohesion.

It is hoped that the findings of this work could clarify the micro-mechanisms of various experimental phenomena such as grain refinement in metals during severe plastic deformation, which can be used to design optimized route of making stabilized bulk NC metals.

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Last but not least, I would like to thank my family with their helps and supports and my friends who encouraged me to overcome the obstacles and make career.

... و کفی بالمرء جهلاً ان لا یعرف قدره ...

... و همین برای جهل آدمی بس که قدر خود را نداند ...

خطبه 102 نهج البلاغه

… and this ignorance is enough for human that he does not know his own value …

… und diese Unwissenheit ist genug für den Menschen, dass er seinen Wert nicht erkennt ...

Sermon 102, Nahjulbalagheh.

امیرالمومنین علی (علیه السلام)

Imam Ali (600-661 A.D.)

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Abbreviations

CLS	Coincidence Lattice Site
CAN	Common Neighbour Atom
DRX	Dynamic Recrystallization
EAM	Embedded Atom Method
ECAP	Equal Channel Angular Press
FCC	Face-Centered Cubic
GB	Grain Boundary
HPT	High Pressure Torsion
MD	Molecular Dynamics
NC	Nanocrystalline
SPD	Severe Plastic Deformation
SAGBM	Shear-Assisted Grain Boundary Motion
SCGBM	Shear-Coupled Grain Boundary Motion
SRX	Static Recrystallization
SDGBM	Stress-Driven Grain Boundary Motion
SUM	Structural Unit Model
TJ	Triple Junction

CHAPTER 1 Motivation and Outline

1.1. Motivation

Grain Boundary (GB) motion and its interaction with other features of materials such as cracks, Triple Junctions (TJs) and dislocations governs the microstructural evolution of every class of polycrystalline materials during deformation and plays important roles in determining the mechanical properties of materials. Therefore, Stress-Driven GB Motion (SDGBM) has been extensively studied in the past [1–9]. The influence of GB and SDGBM is more prominent when the grain size in materials is reduced to nanoscale, as the volume fraction of GBs dramatically increases in Nanocrystalline (NC) materials, which are usually defined as materials with average grain size of less than 100 nm. In the past, SDGBM has been found to play dual roles on the microstructural evolution in NC materials. On one hand, SDGBM can lead to dramatic grain growth in NC materials during mechanical deformation, which would degrade the outstanding mechanical properties in NC materials [10,11]. On the other hand, SDGBM is also believed to influence producing bulk NC metals, *e.g.*, during grain refinement by Severe Plastic Deformation (SPD) [12,13]. It is thus important to explore the atomistic mechanisms of SDGBM and clarify their importance during the deformation of NC materials.

Experimental techniques which give valuable insights about different aspects of material science require expensive facilities and are limited only to special GB types and deformation modes [14,15]. Analytical methods can only apply to problems with various approximates and assumptions [3,16,17], and lack the atomic details which is crucial for the understanding of SDGBM. As a result, atomistic simulations has been used vastly to study GB motion and other

related phenomena due to its accuracy, flexibility and economic efficiency. In this thesis the proposed method to study SDGBM is Molecular Dynamics (MD) simulation [8].

So far past studies on SDGBM by MD simulations were mainly limited to bicrystal models [1,18–21]. In this thesis, the influences of other features of materials such as TJs, cracks, and neighbouring grains on SDGBM will be systematically studied, which has been rarely considered before.

1.2. Objective

In this thesis, MD simulations are used to study GB motion under shear deformation and the interaction of GB with other defects including TJs and nano-cracks in nanocrystalline face-centered cubic (FCC) metals. Specifically this research has three main objectives:

- To systematically compare SDGBM in NC and bicrystal models and study the influences of temperature, GB type and TJs.
- To investigate the atomic mechanisms of interaction between SDGBM and nano-cracks.
- To explore the atomistic mechanisms leading to grain refinement and crack healing during SDGBM in metals.

1.3. Outline

In chapter 2 a thorough literature review is presented. This chapter starts by introducing basic information about GB from geometric point of view and GB models such as Coincidence Lattice Site (CLS), dislocation model, structural unit model and disclination based model. Then it reviews the past studies on SDGBM including those in both bicrystal and polycrystalline models and their influence on grain growth and grain refinement.

In chapter 3 the method used in building and performing simulations are presented. Theory of MD, the method of embedded atom potential and the parameters used are presented.

In chapter 4 the results of this work including systematic comparison of GB motion between bicrystal and NC models, influence of TJ on GB motion, interaction of SDGBM with nano-cracks and the corresponding discussions are presented.

In chapter 5 some important conclusions based on this work are made and some future work suggestions are presented.

CHAPTER 2 Literature Review

2.1. Grain Boundaries

2.1.1. Geometry of Grain Boundaries

The interface between two crystallites or grains of same material with different orientations in a crystalline material in a manner that material is continuous across this interface is called Grain Boundary (GB) [22]. Nine parameters are needed to describe the geometry of a GB uniquely; four are microscopic or energy parameters and five are macroscopic parameters [23]. The energy parameters are defined by nature and we do not have control on them. Three macroscopic parameters in a cubic system are the rotational axis cosines [u v w] (two parameters) and the rotation angle θ(one parameter); the other two define the normal of the interface plane (Miller indices).

With this terminology a GB is said to be tilt if the axis of rotation [u v w] is in the plane of GB, it is twist if the rotation axis [u v w] is perpendicular to GB plane and if the rotation axis is inclined, the GB is called mixed. On the other hand if the plane between two grains can be expressed by$\{h\,k\,l\}_1 = \{h\,k\,l\}_2$, the boundary is called symmetric otherwise it is asymmetric, as shown in Figure 2-1.

The lowest energy is achieved when two adjacent grains have the same orientation, *i.e.*, there is no GB between them. By rotating one grain relative to the other, the energy increases but there are some special angles of rotation, for which the energy is a local minimum [24], Figure 2-2. The reason of this lower energy is that, there are sites on GB which coincide to both adjacent grains. The Coincidence Lattice Site (CSL) theory describes special GBs, which have common lattice sites in GB as shown in Figure 2-3. Based on CSL theory, the misorientation

angle between two grains cannot be any arbitrary value since the free energy becomes high and the material tends to decrease it, so the misorientation angle should be a local minimum to be stable. As a parameter to measure the coincidence sites we define Σ as the fraction of the volume cell of CSL to the volume cell of crystal lattice as in 2-1:

$$\Sigma = \frac{\text{volume cell of CSL}}{\text{volume cell of crystal lattice}} \qquad 2\text{-}1$$

Nevertheless CSL model cannot describe every grain boundary and there are more generalized models such as 0-lattice theory [25,26], which has been employed to model GB for different studies.

Figure 2-1 Relative orientation of GBs and rotation axes for different types of GBs. (a) Twist boundary; (b) asymmetric tilt boundary; (c) symmetric tilt boundary [24].

Figure 2-2 Dependence of the energy of symmetric ⟨110⟩ tilt boundaries in Al on the tilt angle Φ. The indices given in the figure are Miller indices of the corresponding GB planes [24].

Figure 2-3 Coincidence lattice unit cells viewed along the rotation axis (a) of a Σ=5 bicrystal: rotation around the 001 axis in a body-centered cubic lattice; (b) of a Σ=3 bicrystal: rotation around 011 in a face-cantered cubic lattice (here four coincidence cells are represented). The common points of the lattices are bicoloured. Different point sizes indicate different positions along the normal to the scheme. The projection of the crystalline lattices is indicated by dashed lines [23].

2.1.2. Dislocation and Structural Unit Models of GB

In this section two common models to describe the GB by dislocations and structural units are briefly explained.

2.1.2.1. The Read-Shockley Model

Read and Shockley first proposed a model to describe a low-angle grain boundary by means of a wall of discreet dislocations [27]. Based on this model, for example a symmetric tilt GB with misorientation angle of θ is built by edge dislocations with burgers vectors of magnitude b placed with distance d apart from each other (Figure 2-4), therefore we have,

$$\theta = \frac{b}{d} \qquad 2\text{-}2$$

Figure 2-4 Read-Shockley low angle GB model [23].

This model is suitable for low-angle GBs, *i.e.* the misorientation angle is less than 15^{o}. For high-angle GBs, the dislocations become so close that their cores overlap. To generalize the Read-Shockley model, Frank-Bilby [28,29] and 0-lattice by Bollmann [25,26] were introduced. The Frank-Bilby model does not provide information on local states of dislocation but only gives the relationship between burgers vector of dislocations and misorientation angle of boundary and 0-lattice theory does not account for the plane of boundary and is an inherent geometric model, which only correlates the boundary and the misorientation angle between adjacent grains.

2.1.2.2. Structural Unit Model

None of the aforementioned models give any information about the structure and subsequent stress field of the GB. Another approach to investigate GB in more details considering its local microstructure is the Structural Unit Model (SUM) [30]. In this approach, based on the interatomic potential used, the GB is relaxed and the special misorientation angles, at which the GB shows the short-range periodicity is considered as favoured boundaries and these units are called fundamental; any other boundary with an arbitrary misorientation angle within two successive favoured boundaries is consist of the units of them. This approach gives consistent results for both symmetric and asymmetric boundaries and can give information about the local stress field in the boundary plane, as it was unavailable from previous models. It is noteworthy that this model does not give information about the energy of boundary and the favoured boundaries in this model are not necessarily low-index Σ boundaries.

Figure 2-5 shows structural observation and simulation of $\Sigma 11\{332\}$ in nickel and germanium. The key point about SUM is the description of GB in terms of structural units. For example $\Sigma 11\{332\}$ in nickel is constructed of 'E^- D E^+ D' sequence while same GB in germanium is consisted of 'M^+ T M^- T' sequence, Figure 2-5.

Frolov *et al.* have shown recently that by changing the atomic density of GB by adding and removing free volumes caused by point defects, many different phases are observed and GB can transform its structure [31]. They built a simulation box of copper with $\Sigma5(130)$ and $\Sigma5(120)$ and showed by adding interstitials and vacancies the GB structure changes and they claimed this phase transformation is reversible. This finding shows that high-angle GBs can absorb up to certain amount of vacancies. Figure 2-6 shows transformation of $\Sigma5(130)$ from its original structure by adding interstitials then adding vacancies and reaching original structure at 800 K.

Figure 2-5 (a),(d) Observed and (b),(c) simulated atomic structure of the $\Sigma11\ \{332\}$ boundary (a),(b) in nickel and (c),(d) in germanium (b),(d). The white arrows in (a) indicate the presence of extrinsic dislocations [23].

Figure 2-6 Isothermal reversible GB-phase transformations induced by point defects. GB-phase transformations in the Cu $\Sigma5(130)$ GB induced by interstitials and vacancies in a simulation block with periodic boundary conditions at$T = 800$ K. After 80 interstitials are introduced into a 10 Å thick layer containing the GB, (a) it transforms from the initial normal-kite structure (b) to a disordered state (c) and then to split kites. (d) After the subsequent introduction of 80 vacancies into the same GB layer, the split-kite structure disorders and (e) then transforms back to normal kites. The GB states (a) and (e) are identical confirming that the transformation is fully reversible [31].

2.1.3. Disclination Model of GB

Volterra first introduced a special class of rotational dislocations (known as disclinations now) along with translational dislocations (which are known as dislocations now) and these two categories are called distortions as shown in Figure 2-7 [32]. In Figure 2-7, six Volterra distortions are shown. The strength of a dislocation is corresponded to the magnitude of Burgers vector $\boldsymbol{b}$, which is equal to the translational displacement of the non-deformed surfaces of the cut bounded by a dislocation line. In the same sense the strength of a disclination is proportional to the magnitude of an axial vector $\boldsymbol{\omega}$ (Frank vector), which defines the relative rotations of the undeformed surfaces of the cut bounded by a disclination line [33].

Figure 2-7 Volterra distortions in an elastic cylinder: (a) initial undistorted state of a hollow cylinder. (b) Screw dislocation with burger vector $\boldsymbol{b}$ parallel to cylinder axis $\boldsymbol{l}$. (c),(d) Edge dislocations with Burgers vector $\boldsymbol{b}$ perpendicular to the line of defect $\boldsymbol{l}$. (e) Wedge disclination with Frank vector $\boldsymbol{\omega}$ parallel to the line of the defect $\boldsymbol{l}$. (f),(g) Twist disclinations with Frank vector $\boldsymbol{\omega}$ perpendicular to the line of the defect $\boldsymbol{l}$ [33].

After introduction of disclinations, it was assumed that this class of distortions due to their long range elastic stress and hence energy cannot be found in solid materials. By new investigations and observations partial disclinations and disclination dipoles, which is two disclinations with same magnitude and different signs [34], were found in solid materials and by using the disclination concept many features resolved in solid materials [34–38], see for examples in Figure 2-8 to Figure 2-10.

Figure 2-8 Microbands in deformed materials and their disclination interpretation: (a) TEM micrograph of a microband in copper single crystal rolled down to 70% thickness reduction at room temperature, Klemm *et al.* [39]. (b) Schematic showing cell wall junctions with disclination quadrupole configuration [33].

Figure 2-9 Terminated microband equivalent to wedge disclination dipole: (a) TEM image of defect structure in restrained polycrystalline Mo specimen, Luft [40]. (b) Schematics showing partial wedge disclination dipole [33].

Figure 2-10 Hierarchical structure of deformation twins, Müllner and Romanov [41]:(a) TEM of primary twin in austenitic steel with the family of secondary (internal) twins. (b) Schematics showing alternating sign disclination walls along the boundaries of the primary twin [33].

One of the applications of disclination model is to describe GB in terms of a sequence of disclination dipoles [42–45]. Figure 2-11 shows two examples of using disclination theory in modeling a zigzag tilt GB (Figure 2-11(a)) and computing the elastic energy of a compensating triple line (Figure 2-11(b)), respectively.

Figure 2-11 Disclination model of GB. (a) A faceted disclination wall representing the structure of zigzag tilt GB [45]. (b) Using disclinations to model GBs and triple line and to compute the elastic energy of triple line (green hollow triangle) [42].

The two advantages of disclination theory to model the GB in compare to dislocation theory are [45]:

- Due to well-behaviour expression for elastic energy of disclination dipoles, elastic energy of a wider interval of misorientation angles can be obtained.
- The misorientation angle of GB between two successive special boundaries can vary continuously in this theory.

Disclination theory has shown promising ability to describe and model different GB related phenomena such as different GB migration modes, special geometry GB, rough GB and other special geometries such as triple and quadruple lines.

2.2. Shear-Assisted GB Motion

Stress-Driven Grain Boundary Motion (SDGBM), *i.e.*, GB motion due to shear stress acting on the boundary plane, is the main mechanism of microstructural evolution in crystalline materials under deformation and loading [11,46–53]. It has been found that shear-coupled motion, which is the simultaneous motion of GB in both perpendicular and parallel to the boundary, is the main mechanism acting in crystalline metals in grain growth and plasticity under nanoindentation [54–56], tension [57–60] and shear [61,62].

2.2.1. Bicrystal Model

The most fundamental step in studying the GB motion is to investigate a bicrystal model [18]. A bicrystal model is consisting of two grains with a GB between them. Figure 2-12 shows a bicrystal model which is used to study the GB migration under shear stress. The shear stress is imposed on GB plane by fixing the lower slab of atoms and moving the upper slab of atoms in a direction parallel to GB plane, in this way, GB is imposed by a shear stress and shows SAGBM [18].

Figure 2-12 Geometry of the bicrystal model used in studying shear-coupled GB motion [18].

Studies on bicrystal models have provided useful and fundamental information about GBs which are presented below.

2.2.1.1. Shear-Coupled GB Motion

Grain Boundary under shear or normal driving forces shows three different motions, *i.e.,* normal, sliding and shear-coupled motion, as shown in Figure 2-13.

Figure 2-13 Illustration of the mechanical response of (a) a bicrystal with inert markers. Applied tractions can result in (b) shear-coupled migration of the boundary in the bicrystal or (c) sliding at the boundary with no boundary migration normal to the interface. A driving force applied

normal to the boundary can result in (d) shear-coupled migration of the boundary in the bicrystal or (e) migration of the boundary normal to the interface without any lateral motion [21].

Shear-Coupled Grain Boundary Motion (SCGBM) is described geometrically by a coupling factor β which is defined as the fraction of horizontal velocity of GB to its normal velocity [19],

$$v_{||} = \beta v_n \qquad 2\text{-}3$$

It is suggested in [18] that the coupling factor only depends on misorientation angle, θ, of symmetric tilt GBs and follows the Equation 2-4. For those GBs which have misorientation angles near 0°, the coupling factor is positive and we call this mode, mode $\langle 100 \rangle$ and for the boundaries with misorientation angles approaching 90° the coupling factor is negative, however the absolute value of coupling factor for a boundary with misorientation angle of θ is equal to a boundary with misorientation angle of $(90° - \theta)$.

$$\beta_{\langle 100 \rangle} = 2\tan\left(\frac{\theta}{2}\right) \qquad 0 < \theta < 32°$$
$$\beta_{\langle 110 \rangle} = -2\tan\left(\frac{\pi}{4} - \frac{\theta}{2}\right) \qquad 32° < \theta < 90° \qquad 2\text{-}4$$

The coupling factor obtained from bicrystal model for a range of symmetric tilt GBs under both shear deformation [18] and synthetic driving force [21,64] shows very good matching with the theoretical coupling factor described above. However this is an elementary step in studying GB in shear-coupling mode of deformation.

2.2.1.2. Structural Mechanism of Shear-Coupled GB Motion

From structural point of view, the SCGBM is described by the transformation of GB structural units [18]. Figure 2-14 shows the structural units involved in coupled motion of $\Sigma5(120)$ and $\Sigma5(130)$ high-angle GBs. It should be noted that most of the high-angle symmetric tilt GBs are consisted of kite-shaped 'A' units and this unit works in cooperation with 'B' units. In the transition step, an A unit and a B unit will merge and form a double-kite structure and this structure in second step becomes a new A unit and B unit one layer up or down, according to shear direction.

Figure 2-14 Atomistic mechanisms of coupled motion of the (a) $\Sigma5(210)$ and (b) $\Sigma5(130)$ GBs. In both cases B is the lattice structural unit converting to the GB kite unit A. An alternative mechanism for the $\Sigma5(130)$ GB could involve the units A' and B' [18].

This model is expandable to explain the coupled motion of low-angle GBs ($\theta \rightarrow 0°$ or $90°$), for example Figure 2-15 shows the transformation of $\Sigma37(160)$ with misorientation angle of 18.9°. Unit C is interlocked with kite-shape unit A. Atomic rows 1 and 2 are in-plane and out-of-plane atomic rows. If atomic row 1 comes to the same depth with atomic row 2 by $\pm a/2$ along the tilt axis, then by slightly deforming the two units, unit C can transform to unit A.

Figure 2-15 Atomistic mechanism of coupled motion of the Σ37(160) GB. C is the lattice structural unit converting to the GB unit A. 1 and 2 are atomic rows normal to the viewer [18].

2.3. Nanocrystalline Materials

2.3.1. Grain Growth and Grain Refinement

Grain growth takes place to lower the energy of a crystalline material by decreasing the overall energy due to reduced overall GB area. In Nanocrystalline (NC) materials, because of the high GB volume fraction, the tendency to lower the energy by grain coarsening is high; it can take place under loading and deformation even at cryogenic temperatures [56,65]. Thus the outstanding mechanical properties of NC materials such as higher yield and hardness strength and toughness in compare with coarse grained metals that are due to the large volume fraction of interfaces degrade by grain growth [10,11,46–50,66–68]. It is shown that SCGBM is considered as the main mechanism responsible for the grain coarsening in nanocrystalline metals during loading and deformation [51,57,60,61,69,70].

Although deformation usually results in grain growth, there are techniques based on controlled mechanical deformation to produce bulk NC metals which are formed by grain refinement during mechanical deformation. Examples of these techniques, which are classified under Severe Plastic Deformation (SPD), include Equal Channel Angular Press (ECAP) and High Pressure Torsion (HPT), as shown in Figure 2-16 [71].

Figure 2-16 Principles of severe plastic deformation techniques. (a) High-Pressure torsion: a sample is held between anvils and strained in torsion under applied pressure P. (b) Equal channel angular pressing: a work piece is repeatedly pressed through a special die [71].

Figure 2-17 TEM images of ultrafine-grained copper. (a) Copper processed by HPT at room temperature (P = 6 GPa, five turns). (b) Copper processed by ECAP (12 passes) [71].

It is widely accepted that the grain refinement during SPD is due to dislocation activities. Specifically, during high strains and stresses in a crystalline metal, dislocations nucleate and form blocks of dislocations within grains interior [12,71–73]. These dislocations have some metastable cellular structures and by continuing the deformation the relative misorientation between cells increases, leading to the formation of low-angle GBs. Eventually with enough deformation high-angle GBs form, which results in smaller-grain texture, as shown in Figure 2-18 [13].

Figure 2-18 Schematic model of dislocation structure evolution during severe plastic deformation. (a) The formation of dislocation blocks (cellular structure). (b) Transformation to a granular structure. (c) Excess amount of dislocations of same sign remains [13].

2.3.2. Dynamic Recrystallization

Although the dislocation-based model is widely accepted to be responsible for the grain refinement in metals during SPD, recrystallization is also proposed as an alternative approach to study grain refinement and nanocrystallization in metals during mechanical deformation. By definition, recrystallization is the formation and evolution of a new network of grains [74] during deformation and annealing in crystalline metals including metals [75–78] and minerals [79–81]. Recrystallization requires thermally activated processes such as solid state diffusion, which require high enough temperature. Therefor recrystallization requires high thermal energy and occurs during hot working that is called Dynamic Recrystallization (DRX) [74,82,83] or during annealing after cold work that is called Static Recrystallization (SRX) [74,76,78]. Nevertheless, DRX still requires high temperature due to the large activation energy for the nucleation of new grains [83,84].

From microstructural point of view, DRX is observed and modelled generally as follow, Figure 2-19 [74]:

- DRX generally nucleates at old GBs while the grains are undergoing coarsening, where new grains nucleate and cause thickened GBs, Figure 2-19(a) and (b).
- This nucleation continues to happen inside the grains and a ‘necklace’ texture forms, Figure 2-19(c).
- Finally the whole material is fully recrystallized and a new grain network forms, Figure 2-19(d).
- If the grains are not large enough, the difference between former and new grain sizes is not significant, Figure 2-19(e).

Figure 2-19 Evolution of microstructure during DRX. (a)-(d) Large initial grain size. (e) Small initial grain size. The dotted lines show initial GBs [74].

Figure 2-20 shows the GB thickening and new grain nucleation at the old GBs in polycrystalline copper undergone DRX at 400^{o}C.

Figure 2-20 DRX at prior GBs in polycrystalline copper at 400^{o}C, $\dot{\varepsilon} = 2 \times 10^{-2}, \varepsilon = 0.7$ [85].

2.3.3. Role of Triple Junction in GB Motion

Although bicrystal models are successful in studying many fundamental phenomena about GB motion, in real crystalline materials there are other features and constrains such as Triple Junction (TJ) which play important roles specially when the grain size is reduced to $\sim 10\ nm$ and smaller, Figure 2-21. The importance of considering neighbouring grains and TJs increases dramatically when the average grain size decreases to nanoscales, as demonstrated in Figure 2-21 [86]. In NC materials the deformation is governed by GB motion due to high volume fraction of GBs that is reported up to $50\%\ vol$ [87]. King has shown that although TJ is when three grain boundary meets, the characteristics of TJ is different from its constituent GBs [88].

Figure 2-21 The effect of grain size on calculated volume fractions for intercrystalline regions, grain boundaries and triple junctions, assuming a grain boundary thickness Δ of 1 nm [86].

Recently some experimental works on SDGBM in NC materials have been reported [14,60,65,69,89–94]. Rupert *et al.* have shown by testing Al thin film under tension that the shear stress is mainly responsible for grain growth and GB migration [93]. Analytically Dynkin and Gutkin [95] and Bobylev *et al.* [96] by using disclination theory examined GB motion with presence of TJs in symmetric hexagonal and rectangular 2D grain networks and have shown that GB migration is heavily dependent on the geometry of TJs and the shear stress required for GB migration in a hexagonal grain was less than that in a rectangular one. Mesoscale simulation methods including phase field simulations [97–99], Monte Carlo [100–102] and network models [2] have also been used extensively to investigate grain growth in complex systems. Zöllner [102] and Barrales-Mora *et al.* [2] by using Monte Carlo Potts model and network models, respectively, took into account the influence of TJs and quadruple lines on the grain growth in NC materials. However, there are limitations in these studies although they were important in evaluating the microstructural evolution in network of grains. For example, the analytical and mesoscale modeling are highly dependent on the accuracy of important parameters such as boundary and junction mobilities, which can only be fed from atomistic simulations. Furthermore, in the mesoscale studied by Zöllner [102] and Barrales-Mora *et al.* [2], the influences of stress were not considered.

Some works based on MD simulations took into account the influence of grain network and TJs [9,56,103–106]. For example, Velasco *et al*. [103] and Gianola *et al.* [104] used a model consisted of a network of grains and applied strain controlled deformation to investigate the SAGBM. They both showed that in more complex models, in spite of presence of other grains and TJs, the GB showed shear-coupled motion similar to what has been observed in non-constrained bicrystal model but with smaller coupling factor. However, a systematic examination on GB motion in a constrained environment similar to real crystalline materials is still lacking and some of the fundamental issues remain to be examined, *e.g.* how the GB motion would be influenced by neighboring moving GBs in realistic materials and how the GB becomes pinned and unpinned by the TJs, etc.

CHAPTER 3 Methodology

3.1. Classical Molecular Dynamics Method

The aim of computer simulations is to complement our understanding by other methods specially experiments. Figure 3-1 shows schematically the length and time scales of different famous experimental and computational methods. Among these methods, molecular dynamics (MD) is the method of understanding the properties of assemblies of molecules and atoms in terms of the interactions between them in the nano-meter and nano-second scales [107]. In classical MD the goal is to find the microstructure evolution over time by solving a many-body problem and the governing equations are from classical mechanics, specifically Newton's Second Law of Motion. The interaction force between the particles are different functions and called inter-particle potentials. Inter-particle potentials are the most important parameters we can change to achieve accurate enough, yet efficient and possible to implement. The simplest inter-particle potential is the famous Lennard-Jones which describes the force between two particles based on 3-1,

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad 3\text{-}1$$

in which $\varepsilon$is well depth and σ is a finite distance at which the potential is zero.

Figure 3-1 Comparison of different time and length scales for a variety of experimental and computational techniques [108].

By introduction of new computers and reduction of computation costs, the demand for more accurate inter-particle potentials increased. Specifically one of the widest used potentials for metallic materials is the Embedded Atom Method (EAM) potential, in which the force-field is obtained from more accurate methods such as *ab initio* or semi-empirical methods [109]. In this method, in addition to the pair-wise potential, the potential of embedding the atom in its place is also considered as described in 3-2.

$$E = \sum_{i} F_i(\rho_{h,i}) + \frac{1}{2}\sum_{\substack{i,j \\ i \neq j}} \varphi_{ij}(r_{ij}) \qquad 3\text{-}2$$

in which φ_{ij} is the pair-wise potential between particles i and j and F_i is the energy of embedding atom i in the host electron density of $\rho_{h,i}$. These parameters are obtained from other fundamental studies, such as *ab initio* simulations or semi-empirical methods. In this work the used inter-particle potential was EAM.

The general MD algorithm usually has the following steps [110]:

1. Building model: In this step, the geometry, types of atoms and molecules and inter-particle potential are assigned.
2. Initializing: constructed model is not physical, since atoms are at 0 K and there is no force between them, to have a physical model, temperature should be assigned and the system should reach equilibrium before the simulation and any changes are applied. This step is important since if the initializing is not done correctly, the result would not be meaningful.
    a. To assign the temperature, the statistical mechanics is used to have a Gaussian distribution, whose average is the desired temperature. To

achieve it, a distribution of velocity is given to the particles randomly and the temperature is computed by 3-3,

$$3Nk_bT = \sum_{i=1}^{N} \frac{m_i {v_i}^2}{2} \qquad 3\text{-}3$$

in which N is the total number of particles, k_b is the Boltzmann constant, m_i is the mass of i^{th} particle, v_i is the velocity of i^{th} particle and T is the temperature assigned to whole system.

b. Another step which is necessary for simulations, is to give enough time to the system to reach equilibrium and for some specific simulations we might need to find the minimum energy for the configuration, for example as explained in 2.1.1, there are four microscopic parameters to determine the GB which are needed to be found by minimizing the energy.

3. Applying forces or displacements and computing particle trajectories: In this step that is the most time consuming step, any desired boundary changes are applied and using the inter-particle potential the force acting on a particle is computed and then the final position is found using Newton's Second Law. Specifically by solving numerically the 3-4,

$$m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{F}_i = -\vec{\nabla}U(\vec{R}) \qquad 3\text{-}4$$

in which $U(\vec{R})$is the inter-particle potential. At this step any other property of the system can be computed such as Virial stress [111].

4. Step 3 is repeated for as many time steps as desired to finish the time of simulation and the final configuration and properties of the system are determined.

3.2. Parameters and Methods Used in This Thesis

In this work, LAMMPS package for parallel massive MD simulations, which is developed by Sandia National Lab, was used [112]. The EAM potential is used for different materials, namely copper [113], gold [114], nickel [115], aluminum [116] and silver [117] were used. To bring the model to the desired temperature before starting applying the deformation, an isobaric thermostat developed by Nosé and Hoover for $100\,ns$ was applied to the models [118,119]. During the simulation to keep the model at the temperature, canonical NVT thermostat was used. The time step used in this work was $5\,fs$. Atomeye [120] was used to visualize the atomistic configurations and to determine the different crystallographic systems (such as FCC, HPC or stacking faults) Common Neighbour Atom (CNA) [121] method was used. To compute the atomic stresses Virial theorem [111] was applied as follow,

$$\tau_{ij} = \frac{1}{\Omega}\sum_{k\in\Omega}\left(-m^{(k)}\left(u_i^{(k)} - \bar{u}_i\right)\left(u_j^{(k)} - \bar{u}_j\right) + \frac{1}{2}\sum_{l\in\Omega}\left(x_i^{(l)} - x_i^{(k)}\right)f_j^{(kl)}\right) \qquad 3\text{-}5$$

in which k and l are atoms, Ω is the volume of domain, $m^{(k)}$ is the mass of atom k, $u_i^{(k)}$is the i^{th} component of the velocity vector of atom k, $\bar{u}_j$ is the j^{th} component of the average velocity of atoms in the volume, $x_i^{(k)}$ is the i^{th} component of the position of atom k and $f_j^{(kl)}$ is the j^{th} component of the force applied on atom k by atom l.

To apply deformation, two different methods were used in this work. To apply shear two thin slabs of atoms were defined as rigid bodies at the top and bottom of the model. The lower was fixed and the top was moved in the direction parallel to the GB plane in order to apply shear

on the GB, Figure 3-2. For tension, same method was used except that the top moving slab was moved in the direction normal to the GB plane. Another method which used in this research is called synthetic driving force method and was developed by Janssens *et al.* [64]. In this method a grain with a specific orientation is given extra energy and it causes the model to try to decrease its energy so the grain with higher energy is shrunk by grain(s) with lower energy. In this case, the GB between grains with lower and higher energy moves toward the grain with higher energy. This method was successfully applied to bicrystal model to compute the mobility of symmetric tilt GBs in bicrystal models by Homer *et al.* [21].

Figure 3-2 The schematic and atomistic configurations of (a) bicrystal and (b) NC models used in this thesis. Two slabs of atoms at the top and bottom of the models are fixed as rigid bodies. The shear is imposed by translating the upper slab at a constant velocity of $1\ m/s$ while the lower slab is fixed. The horizontal and vertical marker lines are used to indicate the initial and instantaneous GB positions. The atomistic configurations of deformed (c) bicrystal and (d) NC models. The atom colours correspond to the local lattice orientation [122].

CHAPTER 4 Results and Discussion

This chapter is divided into three sections. The first section is about the influences of TJs and network of grains in NC materials on SDGBM, the second section is about a disclination-based micro-mechanism of DRX at low to medium temperatures and the last part is about structural transformation and a new crack healing mechanism by SDGBM found in FCC metals.

4.1. Influences of TJs on SDGBM in NC Metals

4.1.1. SCGBM in NC Metals

The effect of TJs on SCGBM was studied and compared in both bicrystal and NC Cu for two GB types (the GB between grains 1 and 2 in Figure 3-2(b)), *i.e.*, $\Sigma5(120)$ and $\Sigma17(350)$ with misorientation angles of $53.13°$ and $61.93°$ respectively by applying shear deformation in the manner explained in 3.2. Here the. The top slab was moved by $1\ m/s$ in positive X-direction as depicted in Figure 3-2. The boundary conditions of the models were also set as periodic in X- and Y-direction and free surface in Z-direction. The lattice orientation of each grain shown in Figure 3-2(b) is listed in Table 4-1.

Table 4-1 Lattice orientation for each grain in NC model shown in Figure 3-2 for $\Sigma5(120)$ and $\Sigma17(350)$ models.

$\Sigma5(120)$				$\Sigma17(350)$			
	X	Y	Z		X	Y	Z
Grain 1	$[1\bar{2}0]$	$[00\bar{1}]$	$[210]$	Grain 1	$[3\bar{5}0]$	$[00\bar{1}]$	$[530]$
Grain 2	$[\bar{1}20]$	$[001]$	$[210]$	Grain 2	$[\bar{3}50]$	$[001]$	$[530]$
Grain 3	$[100]$	$[010]$	$[001]$	Grain 3	$[100]$	$[010]$	$[001]$
Grain 4	$[1\bar{5}0]$	$[00\bar{1}]$	$[510]$	Grain 4	$[1\bar{3}0]$	$[00\bar{1}]$	$[310]$
Grain 5	$[1\bar{5}0]$	$[001]$	$[\bar{5}\bar{1}0]$	Grain 5	$[1\bar{3}0]$	$[001]$	$[\bar{3}\bar{1}0]$

The vertical and horizontal markers in Figure 3-2 show the path that GB has travelled and the initial position of it, respectively. The coupling factor, β, was computed from the slope of the vertical marker. Despite the constrains in NC model including TJs at two ends of the GB, it still showed SCGBM, which is consistent with previous studies [103,104]. By comparing the shear imposed bicrystal and NC models in Figure 3-2, it is evident that TJs at the ends of the GB in NC model imposed an effect namely "pinning" effect which hindered the GB and caused the GB to curve. From previous studies, it has been shown that the curvature in GB imposes a normal force in the direction of curvature in the sense of inside the curvature, so it is expected that with the same horizontal displacement, the GB in NC model migrates less in the normal direction in compare to the bicrystal model, which could cause the coupling factor to increase according to 2-3 [123]. Another difference is that although there is no dislocation activity observed in bicrystal model, there are dislocation nucleation and propagation in NC model near TJ, whose effects will be discussed in detail in 4.1.7.

4.1.2. Effect of Temperature on SCGBM

From MD simulations on SCGBM in bicrystal models under both shear deformation [18] and synthetic driving force method [21], it has been found that temperature has an important influence on behaviour of SCGBM. In order to investigate the influence of temperature, the temperature of the simulated system varied from 200 K to 800 K with an increment of 100 K and to eliminate the effect of thermal fluctuations each simulation was done four times with different thermal initialization. Figure 4-1 shows atomistic configuration of $\Sigma5(120)$ and $\Sigma17(350)$ NC models at both low temperature ($300\,\mathrm{K}$) and high temperature ($800\,\mathrm{K}$) after $2.5\,ns$ of deformation.

Figure 4-1 Atomistic configurations of NC models for deformed $\Sigma5(120)$ at (a) 300 K and (b) 800 K and $\Sigma17(350)$ at (c) 300 K and (d) 800 K, respectively, after 2.5 ns [122].

$\Sigma5(120)$ in NC model at 800 K has shown almost pure sliding while in our bicrystal model of same GB type no sliding was observed and this agreed with the finding of Cahn *et al.* who reported $\Sigma5(120)$ bicrystal model did not show sliding until 1000 K [18]. This is in contrast to what has been reported by Bernstein that confined GBs showed less sliding and constituent grains showed less rotation in comparison with bicrystal models [124]. On the other hand $\Sigma17(350)$did not show any sliding in either bicrystal or NC models. Furthermore, by comparing each GB type at low and high temperature, it is evident that the $\Sigma5(120)$ GB has stronger temperature dependency than $\Sigma17(350)$ GB.

It is important to note that the TJs have dramatically different pinning effects in these two models. Specifically, TJs show stronger pinning effect, which caused the GB to curve at lower temperature and to slide at higher temperature in $\Sigma5(120)$ model than in $\Sigma17(350)$ model. In addition, although TJs moved along the GB slightly at all temperatures, it is noted that TJs have more significant pinning effect when the temperature is higher.

To quantify the temperature effect on SCGBM with presence of TJs, the coupling factor in all models were obtained by computing the slope of vertical marker line indicated in Figure 3-2, which corresponds to the coupling factor of the center of the GB. The computed β for both NC (green) and bicrystal (red) models and for both GB types, *i.e.*, $\Sigma17(350)$ and $\Sigma5(120)$ are shown in Figure 4-2. The black dashed lines show the theoretical values of β

obtained from 2-4, which are 0.667 for $\Sigma5(120)$ and 0.5 for $\Sigma17(350)$. In contrast to works done by Velasco *et al.* [103] and Schäfer and Albe [9], who found coupling factor to be smaller than theoretical value and value obtained from bicrystal model, here it is shown that β in NC model is higher than theoretical values. This different trend between previous works and this work originates from the loading conditions. In previous works [9,103], NC models were built randomly and were loaded by tension, so the GBs experienced a complex loading while in this work the GB was imposed by pure shear. Further discussions on the apparently larger β in this study are given in Sections 4.1.4 and 4.1.5.

By comparing the coupling factors of bicrystal and NC models with theoretical value for $\Sigma5(120)$ in Figure 4-2, it can be seen that bicrystal model does not show temperature dependency and the coupling factor remains around theoretical value at various temperatures. However, in NC model by increasing the temperature from 500 to 800 K, there is a sharp increase in coupling factor which is due to the more significant sliding behaviour of GB at higher temperature.

Figure 4-2 Coupling factor β, at different temperatures in NC and bicrystal models containing (a) $\Sigma5(120)$ and (b) $\Sigma17(350)$ GBs. The horizontal dashed lines show the theoretical values of β for the corresponding GB type.

4.1.3. Time Dependent Non-Linear GB Motion

In bicrystal model it is assumed that GB migrates linearly in both horizontal and vertical directions, so the computed coupling factor is not time dependent. Nevertheless by measuring the

displacement of GBs in NC models, it is suggested that in real material, GB does not move in a linear manner but in a non-linear one, as shown in Figure 4-3. The curves for both $\Sigma5(120)$at 600 K and $\Sigma17(350)$ at 200 K indicated that the horizontal and vertical velocities tend to increase over time, although the imposed shear was constant. Since it was observed in both GB types and at all temperatures, it seems that it is not dependent on GB type or temperature. The reason for this behaviour is discussed in 4.1.6.

Figure 4-3 Horizontal and normal displacements as functions of time for (a) $\Sigma5(120)$ at 600 K and (b) $\Sigma17(350)$at 200 K in NC models [122].

4.1.4. Effect of Loading Mode on Coupling Factor $\boldsymbol{\beta}$

In 4.1.2 it was shown that the computed coupling factor in NC models in this study is higher than the coupling factor reported in works by Velasco *et al.* [103] and Schäfer and Albe [9] and it was mentioned that the main reason should be the different loading conditions between this work and aforementioned studies. To further investigate the influence of loading mode, synthetic driving force method was used, *e.g.*, an excess energy of $-0.01\ eV/atom$ (equivalent of $-0.14\ GPa$) was added to grain 2 in NC models or the lower grain in bicrystal models at 800 K. To decrease the overall energy of the system, the grain with artificially added negative energy will become bigger by moving the GB upward. The normal position of the goal GB was tracked during the deformation for both NC and bicrystal models for both GB types and are depicted versus time in Figure 4-4. Comparing the bicrystal models with NC models, it is obvious that in general, the GB in bicrystal model moved differently from that in the NC model.

Specifically in NC models due to hindering effects from TJs, the GB migrated less in normal direction for the same time (and hence shear deformation) than in the bicrystal model.

It has been reported in previous bicrystal simulations [18] that $\Sigma5(120)$ GB showed 'stick-slip' behaviour during SCGBM. Here in both bicrystal and NC models, $\Sigma5(120)$ also showed stick-slip behaviour suggesting that this behaviour is the nature of this GB type and is not influenced by other grains or obstacles. The reason for this behaviour is that for $\Sigma5(120)$ GB, the shear stress should reach a threshold in order to start moving while in other GBs, for example here $\Sigma17(350)$, there is much less or no threshold for onset of the SCGBM. This threshold is likely due to the structural changes during SCGBM; for specific structures, there is a higher energy barrier from current structure to transition step, which was discussed in 2.2.1.2.

Figure 4-4 Normal displacement of bicrystal and NC models for (a) $\Sigma5(120)$ and (b) $\Sigma17(350)$ at 800 K. (c) Atomic configuration of $\Sigma5(120)$ NC model at 800 K after 5 ns [122].

As can be seen in Figure 4-4(c), the loading mode has substantial effect on GB motion. By applying the synthetic driving force, unlike the bicrystal model, which showed same SCGBM as shear-induced GB motion in bicrystal model [21], the NC model in this work almost did not show significant coupling motion and in some cases pure normal motion was observed. It can be concluded that unlike coupling factor which was claimed to be a pure geometry parameter and does not depend on loading mode [18,21], it is influenced significantly by loading mode in real NC materials.

Overall by comparing the two NC models, it can be concluded that the stick-slip motion caused the SCGBM more difficult for $\Sigma5(120)$ GB than $\Sigma17(350)$, which moved smoothly as shown in Figure 4-4 [18].

4.1.5. Influence of TJ Pinning on Coupling Factor β

In addition to geometry of the GB and loading mode, which have great influences on the coupling factor in NC materials, other parameters might have influences, too. It was shown in Figure 4-2 that $\Sigma5(120)$ NC model has more deviation from theoretical values of coupling factor in compare to $\Sigma17(350)$ NC model. This deviation can be attributed to the difference between pinning effects of the TJs in those models.

$\Sigma17(350)$ NC model has shown overall less deviation from the theoretical value of coupling factor than $\Sigma5(120)$ NC model; noticeable deviations were only found at $200\ \mathrm{K}$, $500\ \mathrm{K}$ and $800\ \mathrm{K}$, as shown in Figure 4-2. By investigating the atomistic configurations at these temperatures, it was found that the GB curvature is prominent, which resulted in severe hindrance to the normal GB motion and high β (Figure 4-5), while at other temperatures the GB remained almost flat during the deformation. In contrast, GB in $\Sigma5(120)$ NC models became severely curved at all temperatures below $700\ \mathrm{K}$, see Figure 3-2(d) and Figure 4-1(a).

Figure 4-5 Curved GB in $\Sigma17(350)$ NC model (a) after $1.8\ ns$ at $200\ \mathrm{K}$ and (b) after $2.5\ ns$ at $800\ \mathrm{K}$ [122].

4.1.6. Origin of Non-Linear SCGBM in NC Models

In bicrystal models in order to compute the coupling factor, it is assumed that the applied shear is same as the horizontal velocity of the GB, which means that the velocity of the top slab in bicrystal model is the same as $v_{||}$ in 2-3. To validate this assumption in NC model, four different layers of atoms were defined between the GB and the top slab in the Z-direction (the inset of Figure 4-6(a)) and the horizontal velocity of these layers were computed and are shown for $\Sigma 17(350)$ NC model at 800 K and 300 K in Figure 4-6(a). For comparison the same method was used to compute the horizontal velocities of different elevations in $\Sigma 17(350)$ bicrystal model and the result is plotted in the inset of Figure 4-6(b). The result obtained from bicrystal model suggested that the assumption of uniform shear deformation from the top slab to the GB is accurate and at different locations along Z-axis the computed horizontal velocity is the same as the top slab. In contrast to bicrystal models, this assumption does not hold for the NC models; both Figure 4-6(a) and (b) show that the shear deformation increased from the original GB position (layer 1) to the top slab and it is always smaller than the applied shear. By comparing the results at two temperatures, it is evident that the difference in horizontal velocity between different layers is more prominent at lower temperature.

The non-linear velocity profile of GB, which was shown in Figure 4-3 can now be well explained: the shear imposed on the GB increased as it moved upward, which caused both the normal and horizontal velocities to increase with time.

Figure 4-6 Horizontal displacement versus time for four layers of atoms above the GB in the $\Sigma17(350)$model at (a) 800 K and (b) 300 K. The vertical dashed lines indicate the time at which a ‘jump’ in GB displacement occurred. The inset in (a) shows the schematic of the four layers at different locations between the GB plane and the top surface. The inset in (b) shows the horizontal displacement versus time of the same four layers in the $\Sigma17(350)$ bicrystal model at 300 K.

The origin of this non-uniform shear over the Z-axis was investigated by looking carefully at the atomistic configuration of NC models. Figure 4-7 shows upper left part of a deformed $\Sigma17(350)$ NC model at 200 K. In real NC materials under deformation, it is expected that every GB in the system should move depending on the respective stress states. Here we show in Figure 4-7 that although $\Sigma17(350)$ GB between grains 1 and 2 (Figure 3-2(b)) moved up due to shear stress, another GB between grains 3 and 4 moved down under the same shear stress. This opposite movement dragged the grain 4 to the left and thus reduced shear magnitude acting on the model. The arrows in Figure 4-7 show the path that the two GBs have moved.

Since this non-linear motion and non-uniform shear deformation were first observed in this work and are due to the confinements such as TJs and other grains, it should arouse curiosity to investigate these phenomena further for future works.

Figure 4-7 Shear induced motion of different GBs in the $\Sigma17(350)$ NC model at 200 K. The arrows indicate the moving paths of the two GBs [122].

4.1.7. Influences of Dislocation on GB and TJ Motion

In Figure 4-6 a 'jump' in the horizontal position of atomic layers above $\Sigma17(350)$ GB in NC model was recognized at 1.7 ns, which was indicated by a vertical dashed line. To explore the origin of this phenomenon, atomistic configurations of both $\Sigma17(350)$ and $\Sigma5(120)$ NC models were examined before and after the jump. Figure 4-8(a) and (b) show the four atomistic configurations of $\Sigma5(120)$ at 200 K and $\Sigma17(350)$ at 300 K, respectively to show the mechanism of jump. TJ locations were indicated by dashed circles.

As it can be seen for $\Sigma5(120)$ NC model in Figure 4-8(a), at $t = 2.7\ ns$ there is no dislocations and $0.1\ ns$ later some dislocations appeared near both TJs; this dislocation activity caused the right TJ to jump significantly at $t = 3.05\ ns$ and finally at $t = 3.1\ ns$ all the dislocations disappeared. The same mechanism also happened for $\Sigma17(350)$ NC model. At $t = 1.7\ ns$, there is no dislocation involved and after $0.15\ ns$ dislocations appeared near both TJs and the left TJ has jumped up. At $t = 1.9\ ns$ the right TJ also jumped up and at $t = 2.05\ ns$ all the dislocations almost disappeared.

The mechanism explained above suggested that TJs are not as mobile as GB and they need higher energy than GBs to move. The finding of this work that the dislocation appeared prior to TJ movement and is the cause of the TJ jump is in contrast with the report by Legros *et al.*, who have found that dislocation activities followed the grain growth in NC aluminum thin

film [60]. It is clear that the dislocation activities are due to the presence of TJs and neighbouring grains and there is no dislocation involved in bicrystal models.

Figure 4-8 Atomistic configurations of (a) $\Sigma5(120)$ NC model at $t = 2.7$, 2.8, 3.05 and 3.1 ns at 200 K and (b) $\Sigma17(350)$ NC model at $t = 1.7$, 1.85, 1.9 and 2.05 ns at 300 K. The positions of TJs are highlighted by the dashed circles [122].

4.1.8. Asymmetric Pinning Effects of TJs and Generalized SDGBM Mode in NC Materials

By reviewing the atomistic configurations of NC models, it can be observed that there is an asymmetric behaviour regarding the motion of TJs. In better words, one TJ would be less pinned and moved faster and further than the other TJ, which can be found in Figure 4-1(d), Figure 4-5(b) and Figure 4-8. To further investigate the underlying mechanism of pinning and unpinning of TJs, two special $\Sigma5(120)$ bicrystal models with free surface condition along X- and Z-directions were built and deformed by shearing the top and bottom slabs as shown in Figure 4-9. Figure 4-9(a) and (c) show the undeformed models with flat and inclined surfaces, which resemble rectangular and hexagonal TJs, respectively. After 1.25 ns of shear deformation at 200 K, the GB moved up in a coupled manner whereas the left TJ moved almost along GB but the right TJ was pinned, which caused the GB to bend in both models. This is similar to what has been observed in Figure 4-8. The red dashed line in Figure 4-9 shows the hypothetical position of GB if it was not pinned and bent. If the GB was not bent and remained flat, the angle indicated by θ would be the angle between two surfaces of the right TJ. When a TJ has similar angle

between every two neighbour interfaces, *i.e.* 120°, the energy is minimum and more the angle is deviated from this equilibrium angle, more the energy is increased. Here the hypothetical θ between two neighbour surfaces would be more than 180° which is far away from equilibrium and needs a huge energy. It is thus the possible explanation that why the right TJ could not move along the GB: in order to minimize the energy the GB needs to bend and keep a near-equilibrium angle. Same mechanism is expected to act in NC model that does not allow the right TJ to move as free as left TJ due to the high energy barrier in that way.

Figure 4-9 Atomistic configurations of $\Sigma5(120)$ bicrystal models at 200 K (a),(c) undeformed and (b),(d) deformed after $1.25\ ns$. Dashed lines show the GB position if it was completely flat [122].

Based on what we have found in this work, a four-step model to generalize the SDGBM in NC metals with presence of TJs under shear deformation is proposed as shown in Figure 4-10. Upon applying shear deformation parallel to the GB plane, which is confined by two TJs at the ends (Figure 4-10(a)), the GB moves upward (or downward based on the geometry) in a coupling manner but the two TJs are pinned and cause the GB to bend at the beginning of motion (Figure 4-10(b)). Since the energy required for TJs to move are different due to the applied loading mode and the corresponding coupling manner of the GB, the left TJ unpins first and moves along the GB while the right TJ is still pinned (Figure 4-10(c)). As the deformation continues, dislocation starts to nucleate around the right TJ In the last step by providing enough energy, the right TJ moves and catches up with the GB in a ’jump’ manner as shown in

Figure 4-10(d). In this model the transition steps which were missing in proposed model by Bobylev *et al.* [96] are presented. In this work only two special types of symmetric tilt GBs in Cu were studied, because the purpose was to directly compare this study with previous bicrystal works and to investigate the influences of TJs in a systematic way. Here, $\Sigma 5(120)$ was selected as a GB which has stick-slip behaviour and $\Sigma 17(350)$ GB was selected to have smooth motion under shear. However, it should stimulate future works to consider more general GBs and TJs and in other types of metals.

Figure 4-10 Generalized model explaining the GB and TJ motion under shear deformation in NC materials. (a) Initial configuration, (b) both TJs are pinned causing the GB to curve, (c) left TJ is unpinned and (d) both the TJs become unpinned and catch up with the GB [122].

As a comparison with previous experimental results, the four-step model proposed here agrees well with TEM results of SDGBM [60]. Legros *et al.* [60] have observed that during SDGBM of aluminum NC thin film, a grain could grow locally and form a 'nose' shape. This confirms very well our finding on non-uniform motion of different parts of GB which was shown schematically in Figure 4-10(c).

4.2. Disclination Mediated DRX in Metals

By examining the atomistic configurations of the simulated NC models during SDGBM, an interesting phenomenon was observed that a new sub-grain formed due to the asymmetric pinning effects of the TJs. This observation motivated a more detailed work on the mechanisms of grain refinement and dynamic recrystallization (DRX) in NC metals.

4.2.1. Dynamic Recrystallization in NC Copper

A quasi 3D NC model of copper, as shown in Figure 4-11(a), was built to investigate the DRX mechanism during shear deformation. The boundary condition in X- and Y-directions is periodic and in Z-direction is free surface. To apply shear, the top thin slab of atoms were pulled in the positive X-direction by the velocity of $1\ m/s$ while the lower slab was fixed. The lattice orientation of each grain, which is indicated in Figure 4-11(a), is tabulated in Table 4-2. The temperature of simulation was set to $200\ \mathrm{K}$ and the model was relaxed for $0.1\ ns$ before applying deformation. Due to SDGBM, the GBs moved in different ways. In particular, the GB between grains 1 and 2 moved down and because of the pinning effect of the two TJs at its ends, the GB bent near the right TJ. Figure 4-11(b) shows the model after $1.5\ ns$ equivalent to shear strain $\gamma = 7.6\%$.

Figure 4-11 The DRX process in a honeycomb nanocrystalline model of copper under shear deformation at $T = 200\ \mathrm{K}$. (a) The initial configuration, (b) the configuration showing the nucleation of the new sub-grain at $1.5\ ns$ or 7.6% shear strain, (c) the configuration showing the rotation of the newly formed sub-grain at $1.8\ ns$ or 9.1% shear strain. (d)-(e) The schematic model describing the low-temperature DRX process mediated by disclinations. The insets in (b) and (c) show the zoomed view of the new sub-grain, and the solid and open triangles in (e) and (f) show the disclination characteristics of the TJs and the bulged GB.

According to [3,125,126], partial disclinations usually form at the end of a terminated GB or a non-compensated TJ(a TJ with disclination characteristics) [26]. Therefore, the bent GB would lead to the formation of a partial disclination at the bending point as indicated in

Figure 4-11(b). This partial disclination with the disclination located at the original TJs formed a triple-pole disclination which imposed a strong torsion on the surrounded area and caused the atoms to rotate clockwise up to $5°$ as indicated in the magnified inset of Figure 4-11(b). The strength of the disclination triple-pole and the rotation of the surrounded area increased with further deformation until a sub-grain was formed. The newly formed GB transformed the disclination triple-pole to a disclination quadrupole which is more stable and has lower energy. The same mechanism was observed at 400 K.

It is important to emphasize that during this process no dislocations appeared and the first dislocations appeared at $t = 2.4\, ns$ that is after new grain was formed. Based on this result we propose a model for disclination based low-temperature DRX mechanism, which is shown in Figure 4-11(d)-(f). In Figure 4-11(d) a network of hexagonal grains with six TJs is under shear deformation. Due to shear coupling effects, the GBs will move as having been explained in previous sections. Assuming that the top GB moves down and since it is dragged by the two TJs at its two ends, it bulges. In addition to pinning effect of TJs, as it was shown in [122], two TJs at the two ends of a GB show asymmetric pinning effect. In this case, the left TJ moves along GB while the right TJ pinned and does not move (Figure 4-11(e)). The bending of GB causes the strength of the right TJ to increase significantly and leads to the formation of a partial disclination at the bending point. These two disclinations along with the disclination of another neighbouring TJ, which is indicated by a white triangle, form a triple disclination region. This triple-pole disclination imposes a strong torque on the surrounding area, which causes the atoms to rotate and eventually a new low-angle GB to form. By forming this new GB, another TJ and disclination forms, which produces an asymmetric disclination quadrupole that has much lower energy than previous configuration (Figure 4-11(f)).

Table 4-2 The lattice orientation of each grain indicated in Figure 4-11(a).

Grain number	X	Y	Z
1	$[100]$	$[010]$	$[001]$
2	$[1\bar{3}0]$	$[00\bar{1}]$	$[310]$
3	$[1\bar{3}0]$	$[001]$	$[\bar{3}\bar{1}0]$
4	$[3\bar{5}0]$	$[00\bar{1}]$	$[530]$
5	$[\bar{3}50]$	$[001]$	$[530]$

4.2.2. Disclination-Mediated DRX in Cu Bicrystal

To further investigate the cooperation of SDGBM and constrains such as TJ, which resulted in DRX, it was necessary to consider other common constrains in metals such as cracks and precipitates. Bicrystal models of $\Sigma 17(350)$ GB including a crack with size of $4 \times 2\ nm$ (Figure 4-12(a)-(c)) and a precipitate (a fixed group of atoms that moved as a rigid body) (Figure 4-12(d)-(f)) ahead of the GB were built and underwent shear deformation in the same way as indicated in Figure 4-11(a) at 10 K.

After applying the shear for $5.3\ ns$ the GB was hindered by the crack and thus bulged and pinned at the two upper crack corners. By this configuration due to the bends in GB, four partial disclinations were produced and formed an asymmetric disclination quadrupole, which are indicated as black and white triangles in Figure 4-12(b). The σ_{zz} component of stress state in the inset of Figure 4-12(b) indicates the formed asymmetric disclination quadrupole on top of crack and GB. Upon further deformation the GB tended to move upward while pinned by crack corners caused the bent part of GB to rotate, which would increase the strength of disclinations and the overall energy of the system. By reaching a certain threshold of strain energy accumulated in the system, the atoms surrounded by disclination quadrupole rotated dramatically. This rotation caused the orientation of those atoms to change and formed a new sub-grain, as shown in Figure 4-12(c). The inset of Figure 4-12(c) clearly indicates the rotation of atoms

during the formation of the new sub-grain. The same mechanism was found in the interaction of $\Sigma 17(350)$ with a rigid obstacle in Figure 4-12(d)-(f). When the GB reached the obstacle, it bent and formed an asymmetric disclination quadrupole, whose stress distribution is shown in the inset of Figure 4-12(e). By continuing the deformation and when the energy of the system reached a threshold, the atoms rotated and formed a sub-grain. Furthermore, the inset of Figure 4-12(f) shows the deformation twinning of the formed sub-grain.

Figure 4-12 The process of DRX mechanism in bicrystal models with (a)-(c) a crack and (b)-(d) a rigid obstacle. (a),(d) Initial configurations. (b),(c) Formation of an asymmetric disclination quadrupole and the corresponding distributions of stress σ_{zz}. (c),(f) Nucleation of the new grains. The inset in (c) indicates the rotation of atoms prior to formation of sub-grain and the inset of (f) shows the twinning in the new sub-grain.

Although SDGBM and disclination were not commonly correlated in literature to model grain refinement, there are some analytical disclination-based models explaining grain refinement in SPD [34,127–130]. For example Orlova *et al.* [16] have proposed that formation of an asymmetric disclination quadrupole causes the atoms inside it to rotate so that two diagonal boundaries will form. With further rotations four sub-grains will eventually form. However, there are some key differences between the work by Orlova *et al.* and the mechanism presented here. First the emphasis on the role of SDGBM to form disclination quadrupole is different. In the work by Orlova *et al.*, it is proposed that a disclination quadrupole is formed but they assumed it is the geometry of a rectangular grain, while in present work, we showed that how SDGBM facilitated formation of a disclination quadrupole. Second the uniform rotation which

has observed here caused the whole region to rotate and form a new sub-grain, while in disclination model proposed by Orlova *et al.*, they assumed two diagonal dislocation walls form inside the disclination quadrupole and four regions form and rotate until four sub-grains form.

4.2.3. Disclination-Mediated DRX in General SDGBM in Copper

To investigate the generalization of the disclination-mediated DRX mechanism, two more loading modes were considered. For this purpose a bicrystal model for tensile loading (Figure 4-13(a)) was built and the synthetic driving force method was applied to the previous bicrystal model (Figure 4-13(c)). In the tensile bicrystal model, a 45° inclined $\Sigma 17(350)$ GB was constructed in the middle and the tensile deformation was applied at 10 K by fixing the lower slab of atoms and moving the top lab of atoms upward. This configuration would impose shear stress on the GB plane. A circular void of 2 nm in diameter was created ahead of the GB which caused the GB to bend. Due to the bending of the GB, a quadrupole disclination was formed and eventually a new sub-grain was nucleated due to the rotation of atoms within it (Figure 4-13(b)). On the other hand, synthetic driving force method was applied in the model as shown in Figure 4-13 (c) by adding $-0.015\ eV/atom$ to the lower grain at 600 K, which showed the same DRX mechanism by GB bulging and atom rotation(Figure 4-13(d)). The latter result also confirms that this mechanism is viable to occur at relatively higher temperatures.

Figure 4-13 (a) Undeformed and (b) deformed bicrystal model with void under tension at 10 K. (c) Undeformed and (d) deformed bicrystal model with crack imposed by synthetic driving force of $0.015\ eV/atom$ at 600 K.

4.2.4. Atomistic Mechanisms of DRX in Copper

The detailed mechanisms of the intermediate steps between Figure 4-12(b) and Figure 4-12(c) are shown in Figure 4-14 . Shockley partial dislocations were nucleated and propagated in both directions inside the area surrounded by disclination quadrupole at the beginning of rotation process, Figure 4-14(a) and (b). It should be noted that these dislocations were not nucleated from crack boundaries or GB, which are the normal dislocation nucleation sites, but inside the area due to rotation caused by the asymmetric disclination quadrupole. This distinction is the main and clarifying point of mechanism proposed here in comparison with previous dislocation mechanisms proposed for SPD [12] and DRX [131] which claimed that dislocations were origin of new grain formation rather than product of it.

Upon further rotation, another set of partial dislocations nucleated and transformed the partial dislocations into coherent twin boundaries along {111} planes, Figure 4-14(c). The same mechanism was observed at higher temperatures, *i.e.* 400 K and with both crack and rigid obstacle. The observed mechanism here is in good agreement with previous analytical models on disclination-based twinning in metals [36,132] and that the formation of coherent twin boundaries after dislocation nucleation significantly reduces the strain energy of the material [133] thus facilitating formation of new sub-grains.

Figure 4-14 Detailed atomistic mechanisms of atom rotation and new grain nucleation in the bicrystal model with a crack under shear deformation. (a) Dislocation nucleation at the onset of

atom rotation, (b) propagation of the nucleated partial dislocations and (c) twinning upon further rotation.

The bulging and 'serration' of the moving GB in confrontation with obstacles, which was observed in this work in bicrystal models presented here is consistent with the observed serrated GB due to SDGBM in $Al-0.5\%Mg$ [134], however we emphasize that the mechanism presented here is a disclination-based rather than dislocation-mediated and furthermore, in contrast to the experimental observation of sub-grain formation with only twin boundaries in copper bicrystal under tension reported by Miura *et al.* [135] the mechanism of this work involves general GBs.

Cracks, precipitates and TJs are common features of crystalline metals, hence it is expected that the disclination-mediated DRX mechanism presented here has significant influence on microstructural evolution of crystalline metals under deformation at low to medium temperatures. For example, the disclination-mediated DRX should dominate the grain refinement regime of early stages in SPD when SDGBM is activated but the dislocations are not significantly involved.

4.2.5. Energy Favourability of DRX in Copper

As any material in nature tends to reduce its energy, the energy favourability of the disclination-mediated DRX mechanism was examined in terms of strain energy of the whole model. The elastic strain energy of each atom was calculated using **Error! Reference source ot found.**and averaged over whole model,

$$E = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \quad 4\text{-}1$$

in which C_{ijkl} are elastic constants from [20] and ε_{ij} and ε_{kl} are strains with $i, j, k, l = 1 - 3$.

As an example, the average elastic energy of the bicrystal model embedding a crack (Figure 4-12(a)) is computed before and after the sub-grain formation and is plotted against time in Figure 4-15. As shown in this figure, the energy of the system increased monotonically until it reached a threshold value of ~2.4 MPa, then the energy dropped significantly to ~1.6 MPa in only 0.1 ns, which corresponded to the sub-grain formation. This 0.8 MPa drop in the energy of the system is comparable to 1 MPa, which is in the order of usual GB energy per unit area [24]. This observation is in excellent agreement with the suggestion by Poliak and Jonas [136] that DRX occurs at any temperature when the local energy reaches a maximum and dissipation rate reaches a minimum.

Figure 4-15 Time evolution of the average elastic strain energy of the bicrystal model containing a crack under shear deformation.

4.3. Crack Healing by SDGBM and Structural Transformation

While SDGBM with the presence of a crack may lead to DRX and the formation of new grains, this mechanism strongly depends on the GB and metal type. In this section, the interaction of SDGBM and cracks with a few more types of GBs and metals is investigated and a new crack healing mechanism is presented.

4.3.1. Influence of Temperature on Crack Healing

A series of bicrystal models each containing an elliptic crack have been constructed and were deformed under shear. Figure 4-16(a) shows the atomistic configuration of copper bicrystal model containing $\Sigma 29(370)$ GB with misorientation angle of $\theta = 46.4°$ and an elliptic crack with length of $5.2\ nm$. The model was shear deformed at different temperatures for $10\ ns$ and due to SDGBM, the GB migrated upward in a coupled manner. It was observed that the interaction of SDGBM with the same crack at different temperature can show three different mechanisms, namely, sub-grain formation, decohesion and crack healing. It is also found that by increasing the temperature the crack healing mechanism predominated other mechanisms.

Specifically it was found that at 10 K after $10\ ns$, the GB was pinned by the crack and became wavy. As similar to DRX mechanism found in 4.2, two sub-grains with dislocations and deformation twins were formed in the lower grain as shown in Figure 4-16(b). For the model deformed at 300 K, the GB showed less serration and the crack propagated along the GB leading to GB decohesion as seen in Figure 4-16(c). More details on decohesion of GB is discussed further in 4.3.5. When the temperature was increased to 500 K, it was observed that the SDGBM interacted with crack, caused the crack to heal and a serrated GB was left upon the completion of crack healing, as shown in Figure 4-16(d).

Figure 4-16 $\Sigma 29(370)$ bicrystal model containing elliptic crack imposed by shear deformation. (a) Undeformed model, deformed (b) at 10 K after $10\ ns$, (c) at 300 K after $10\ ns$ and (d) at 500 K after $6.7\ ns$.

4.3.2. Mechanism of Crack Healing in Bicrystal with SDGBM

The atomistic details of crack healing under SDGBM in copper $\Sigma 29(370)$ bicrystal model at $500\ \mathrm{K}$ is illustrated in Figure 4-17. The GB first migrated and reached the crack by SDGBM. Due to asymmetric pinning effect, which was introduced in 4.1.8, the left pinned point remained at lower part of the crack but the right pinned point moved further up, which transformed the originally elliptical crack to an irregular shape with sided facets. The lower grain moved to left and the upper grain moved to right, due to applied shear deformation. Since upper and left sides of the crack belong to upper grain, they moved to right and the right and lower sides of the crack, which belong to lower grain, moved to left and caused the crack to become smaller and finally to heal.

The free volume of the crack is absorbed by the GB by an interesting transformation of the GB plane. Specifically, the GB plane changed from the original symmetric tilt GB to become an asymmetric tilt GB, as shown in Figure 4-17(b). This transformation can accommodate the absorption of free volumes in two different ways. First, the total area of the GB region increased, which can help absorb more free volume. Second, the transformation of the GB plane also dramatically changes the structural units of the GB, which could also host more free volumes. More details about the GB transformation and its influences on free volume absorption is discussed further in 4.3.5.

Figure 4-17 Mechanism of crack healing in interaction with SDGBM. (a) GB showed asymmetric pining effect upon reaching the crack due to SDGBM. (b) Due to SDGBM and

pinning effect the plane of GB changed and the symmetric GB became asymmetric GB. The inset of (b) shows the thickening of GB due to free volume absorption.

4.3.3. Influence of GB Types on the Interaction of SDGBM and Crack

To investigate the influence of GB type, copper bicrystal models were built and simulated at $500\,\mathrm{K}$ containing high-angle symmetric tilt GBs: $\Sigma29(370)$, $\Sigma53(270)$, $\Sigma5(120)$ and $\Sigma5(130)$ with misorientation angles of 46.4°, 31.9°, 53.1° and 36.9°, respectively (Figure 4-18).

In these four GB types, although the temperature and materials were kept the same, three different mechanisms were observed, namely, crack healing without and with dislocation activities for $\Sigma29(370)$ and $\Sigma53(270)$, grain refinement (DRX) for $\Sigma5(120)$ and GB decohesion for $\Sigma5(130)$. The dependency of GB type on the dominating mechanisms may originate from either the difference in geometry, mobility or coupling factor of those grains, which needs an extensive separate research to be explored and is a direction for future work.

Figure 4-18 Influence of GB type. Copper bicrystal models at $500\,\mathrm{K}$ (a) with $\Sigma29(370)$ after $6.6\,ns$, (b) with $\Sigma53(270)$ after $9.15\,ns$, (c) with $\Sigma5(120)$ after $10\,ns$ and (d) with $\Sigma5(130)$ after $10\,ns$.

4.3.4. Influence of Material on the Interaction of SDGBM and Crack

In Figure 4-19 $\Sigma29(370)$ models with different types of FCC metals deformed at $500\,\mathrm{K}$ are shown. Decohesion is more prominent in metals with higher stacking fault energies such as aluminum and nickel as shown in Figure 4-19(b) and (e). In these two models we observed cleavage at almost every temperature and with any GB type that we have studied. Among three

low to medium stacking fault energy metals, *i.e.*, copper, gold and silver, they all showed crack healing mechanism except for silver, which showed partial decohesion (Figure 4-19(a), (c) and (d)). In silver model, the crack shrank but the left tip of the crack propagated along the GB simultaneously. Based on these results, we concluded that stacking fault energy plays an important role on the competition between different mechanisms and for higher stacking fault energy we expect cleavage to prevail over other mechanisms even at considerably high temperatures.

Figure 4-19 Influence of material on the interaction of crack and SDGBM. Models of $\Sigma 29(370)$ and ran at 500 K. (a) Silver, (b) aluminum, (c) gold, (d) copper, (e) nickel.

4.3.5. Structural Behaviour of GB in Crack Healing and Decohesion

As discussed in 4.3.3, GB type has an important influence on the competition between decohesion, crack healing and grain refinement mechanisms. To further investigate the GB in interaction with crack from structural point of view and gain a better understanding of the difference between crack healing and GB decohesion, the detailed atomistic configurations of $\Sigma 5(130)$ in aluminum at 10 K and $\Sigma 5(120)$ in copper at 300 K are shown in Figure 4-20. These two models are representative for GB decohesion and crack healing, respectively, during SDGBM with the presence of cracks. $\Sigma 5(130)$ is originally consisted of discontinuous structural 'A' units which is shown by solid black lines in the flat left part of GB in Figure 4-20(a)-(c). As the GB is pinned at crack and the GB plane has rotated due to pinning effect, the structural units of $\Sigma 5(130)$ GB in the inclined part of GB has changed to continuous A units which are two by

two and back to back. It should be also noted that the GB plane has rotated and its normal is in the same direction of upper grain orientation. These two changes caused the GB in declined part to be ready to open like a ‘zipper’. Figure 4-20(a)-(c) show the ‘unzipping’ process of structural unit labeled as ‘1’ back to back to the structural unit labeled as ‘2’. As the shear deformation continued, unit 1 unzipped completely and the flat part of GB moved one layer up.

Figure 4-20 Detailed atomistic structures of (a)-(c) decohesed $\Sigma5(130)$ aluminum at 10 K and (d)-(f) crack healed $\Sigma5(120)$ copper at 300 K.

On the other hand, the crack healing mechanism is shown in Figure 4-20(d)-(f) for $\Sigma5(120)$ in copper deformed at 300 K. The original $\Sigma5(120)$, which is consisted of continuous A units is indicated in flat part of GB by black solid lines. As structural transformation happened in GB to absorb free volume of the crack, constitutive atoms of GB have been shuffled and they have lost their original structure. This chaos caused the GB not to be able to unzip as was shown for decohesion in Figure 4-20(a)-(c). Nevertheless the GB was also able to form a structure the same back to back A units as in Figure 4-20(b). One example is shown in Figure 4-20(d) by solid black lines in the inclined part of the GB. As the time passed and more free volume is absorbed by GB, the structural units disappeared and the GB became thickened and more shuffled. The key difference between decohesion and crack healing mechanism is the ability of GB to transform phase and absorb the free volume from the crack and shuffle the original structure that hinders the crack to propagate along the GB. This is consistent with work by Frolov *et al.* who reported that $\Sigma5(120)$ transforms suddenly at 400 K while $\Sigma5(130)$ transforms gradually up to

melting temperature. The underlying mechanism that is responsible for structural phase transformation should be investigated carefully in future works.

CHAPTER 5 Summary

Molecular Dynamics simulations were used to study stress-driven grain boundary motion in presence of triple junctions and neighbouring grains in nanocrystalline models. The influences of temperature and TJs were investigated systematically in the first part. In second part, a new low to medium temperature DRX mechanism was found and characterized in NC and bicrystal models. In the last part, the mechanism of crack healing and its competition with decohesion was examined in bicrystal models. Overall, the following conclusions can be made:

- The loading mode has an important influence on SDGBM in presence of TJs, while in bicrystal models this influence is trivial.
- Under shear deformation, the coupling factor of GB is higher in NC models than in bicrystal models because of the pinning effects of TJs. In particular, the pinning effects of TJs are found to be asymmetric depending on the mode of SDGBM.
- Due to influences of other GBs and grains, SDGBM is non-linear in both horizontal and normal directions in NC model.
- Asymmetric disclination quadrupole which is formed during constrained SDGBM by TJs, cracks or precipitates can lead to DRX, or the formation of new sub-grains.
- The disclination-mediated DRX mechanism is found to be independent of temperature and loading mode, which may govern the grain refinement that occurs in early stages of SPD even at cryogenic temperatures.
- A new crack healing mechanism is found in FCC metals which is facilitated by the interaction of SDGBM and crack which is more liable to occur at higher temperatures and in metals with relatively low stacking fault energy.

Findings of this work should enlighten and stimulate potential future experiment and simulation works on confined SDGBM and the interaction of GB with natural features of real materials such as crack and precipitates.

Based on the works presented in this thesis, three journal papers and one conference talk are produced,

- *Influences of triple junctions on stress-assisted grain boundary motion in nanocrystalline materials*, Mohammad Aramfard and Chuang Deng, Modelling and Simulations in Materials Science and Engineering, 2014, 22, 055012.
- *Disclination mediated dynamic recrystallization in metals at low temperature*, Mohammad Aramfard and Chuang Deng, Scientific Reports, accepted.
- *Interaction of stress-driven grain boundary motion with crack: crack healing, decohesion and sub-grain formation*, Mohammad Aramfard and Chuang Deng, manuscript in preparation.
- *Influence of triple junctions on shear-coupled grain boundary motion*, Mohammad Aramfard and Chuang Deng, Materials Science and Technology, 2013, Montreal, QC, Canada.

Bibliography

[1] Péron-Lührs V, Sansoz F and Noels L 2014 Quasicontinuum study of the shear behavior of defective tilt grain boundaries in Cu *Acta Mater.* **64** 419–28

[2] Barrales-Mora L A, Gottstein G and Shvindlerman L S 2012 Effect of a finite boundary junction mobility on the growth rate of grains in two-dimensional polycrystals *Acta Mater.* **60** 546–55

[3] Bobylev S V, Morozov N F and Ovid'ko I A 2010 Cooperative Grain Boundary Sliding and Migration Process in Nanocrystalline Solids *Phys. Rev. Lett.* **105** 055504

[4] Godiksen R B, Trautt Z T, Upmanyu M, Schiøtz J, Jensen D J and Schmidt S 2007 Simulations of boundary migration during recrystallization using molecular dynamics *Acta Mater.* **55** 6383–91

[5] Caillard D, Mompiou F and Legros M 2009 Grain-boundary shear-migration coupling. II. Geometrical model for general boundaries *Acta Mater.* **57** 2390–402

[6] Gottstein G, Molodov D A and Shvindlerman L S 1998 Grain Boundary Migration in Metals: Recent Developments *Interface Sci.* **6** 7–22

[7] Deng C and Schuh C A 2011 Atomistic Simulation of Slow Grain Boundary Motion *Phys. Rev. Lett.* **106** 045503

[8] Mendelev M I, Deng C, Schuh C A and Srolovitz D J 2013 Comparison of molecular dynamics simulation methods for the study of grain boundary migration *Model. Simul. Mater. Sci. Eng.* **21** 045017

[9] Schäfer J and Albe K 2012 Competing deformation mechanisms in nanocrystalline metals and alloys: Coupled motion versus grain boundary sliding *Acta Mater.* **60** 6076–85

[10] Gleiter H 2000 Nanostructured materials: basic concepts and microstructure *Acta Mater.* **48** 1–29

[11] Wolf D, Yamakov V, Phillpot S R, Mukherjee A and Gleiter H 2005 Deformation of nanocrystalline materials by molecular-dynamics simulation: relationship to experiments? *Acta Mater.* **53** 1–40

[12] Estrin Y and Vinogradov A 2013 Extreme grain refinement by severe plastic deformation: A wealth of challenging science *Acta Mater.* **61** 782–817

[13] Valiev R Z, Islamgaliev R K and Alexandrov I V 2000 Bulk nanostructured materials from severe plastic deformation *Prog. Mater. Sci.* **45** 103–89

[14] Protasova S ., Gottstein G, Molodov D ., Sursaeva V . and Shvindlerman L . 2001 Triple junction motion in aluminum tricrystals *Acta Mater.* **49** 2519–25

[15] Gorkaya T, Molodov D A and Gottstein G 2009 Stress-driven migration of symmetrical 〈1 0 0〉 tilt grain boundaries in Al bicrystals *Acta Mater.* **57** 5396–405

[16] Orlova T S, Nazarov A A, Enikeev N A, Alexandrov I V, Valiev R Z and Romanov A E 2005 Grain size refinement due to relaxation of disclination junction configurations in the course of plastic deformation of polycrystals *Phys. Solid State* **47** 845–51

[17] Bobylev S ., Gutkin M Y and Ovid'ko I . 2004 Transformations of grain boundaries in deformed nanocrystalline materials *Acta Mater.* **52** 3793–805

[18] Cahn J W, Mishin Y and Suzuki A 2006 Coupling grain boundary motion to shear deformation *Acta Mater.* **54** 4953–75

[19] Cahn J W and Taylor J E 2004 A unified approach to motion of grain boundaries, relative tangential translation along grain boundaries, and grain rotation *Acta Mater.* **52** 4887–98

[20] Schönfelder B, Wolf D, Phillpot S R and Furtkamp M 1997 Molecular-Dynamics Method for the Simulation of Grain-Boundary Migration *Interface Sci.* **5** 245–62

[21] Homer E R, Foiles S M, Holm E A and Olmsted D L 2013 Phenomenology of shear-coupled grain boundary motion in symmetric tilt and general grain boundaries *Acta Mater.* **61** 1048–60

[22] Hirth J P and Lothe J 1982 *Theory of Dislocations* (Krieger Publishing Company)

[23] Priester L 2013 *Grain Boundaries and Crystalline Plasticity* (John Wiley & Sons)

[24] Gottstein G 2010 *Grain boundary migration in metals: thermodynamics, kinetics, applications* (Boca Raton: Taylor & Francis)

[25] Bollmann W 1970 *Crystal defects and crystalline interfaces* (Springer-Verlag)

[26] Bollmann W 1989 Triple-line disclinations in polycrystalline material *Mater. Sci. Eng. A* **113** 129–38

[27] Read W T and Shockley W 1950 Dislocation Models of Crystal Grain Boundaries *Phys. Rev.* **78** 275–89

[28] Anon 1955 *Defects in crystalline solids: Report of the conference on defects in crystalline solids held at the H.H. Wills Physical Laboratory, University of Bristol, July 1954* (s.l.)

[29] Anon 1950 *A Symposium on the Plastic Deformation of Crystalline Solids: Mellon Institute, Pittsburgh, 19, 20 May 1950* (U.S. Government Printing Office)

[30] Sutton A P and Vitek V 1983 On the Structure of Tilt Grain Boundaries in Cubic Metals I. Symmetrical Tilt Boundaries *Philos. Trans. R. Soc. Lond. Math. Phys. Eng. Sci.* **309** 1–36

[31] Frolov T, Olmsted D L, Asta M and Mishin Y 2013 Structural phase transformations in metallic grain boundaries *Nat. Commun.* **4** 1899

[32] Volterra V 1907 Sur l'équilibre des corps élastiques multiplement connexes *Annales scientifiques de l'Ecole Normale superieure* vol 24 (Société mathématique de France) pp 401–517

[33] Romanov A E and Kolesnikova A L 2009 Application of disclination concept to solid structures *Prog. Mater. Sci.* **54** 740–69

[34] Romanov A and Vladimirov V 1992 Disclinations in crystalline solids *Dislocations Solids* **9** 191

[35] Klimanek P, Klemm V, Romanov A E and Seefeldt M 2001 Disclinations in Plastically Deformed Metallic Materials *Adv. Eng. Mater.* **3** 877–84

[36] Müllner P and Romanov A E 1994 Between dislocation and disclination models for twins *Scr. Metall. Mater.* **31** 1657–62

[37] Romanov A E 2003 Mechanics and physics of disclinations in solids *Eur. J. Mech. - ASolids* **22** 727–41

[38] Romanov A E, Kolesnikova A L, Ovid'ko I A and Aifantis E C 2009 Disclinations in nanocrystalline materials: Manifestation of the relay mechanism of plastic deformation *Mater. Sci. Eng. A* **503** 62–7

[39] Klemm V, Klimanek P and Motylenko M 2002 Transmission electron microscopy analysis of disclination structures in plastically deformed metals *Mater. Sci. Eng. A* **324** 174–8

[40] Luft A 1991 Microstructural processes of plastic instabilities in strengthened metals *Prog. Mater. Sci.* **35** 97–204

[41] Müllner P and Romanov A E 2002 Modeling Internal Twinning with Disclinations and Somigliana Dislocations *Solid State Phenom.* **87** 239–44

[42] Upadhyay M, Capolungo L, Taupin V and Fressengeas C 2011 Grain boundary and triple junction energies in crystalline media: A disclination based approach *Int. J. Solids Struct.* **48** 3176–93

[43] Gutkin M Y and Dynkin N K 2012 Dislocation-disclination models of grain boundary migration in ultrathin nanocrystalline films *Phys. Solid State* **54** 798–807

[44] Gertsman V Y, Nazarov A A, Romanov A E, Valiev R Z and Vladimirov V I 1989 Disclination-structural unit model of grain boundaries *Philos. Mag. A* **59** 1113–8

[45] Nazarov A A, Shenderova O A and Brenner D W 2000 On the disclination-structural unit model of grain boundaries *Mater. Sci. Eng. A* **281** 148–55

[46] Sutton A P and Balluffi R W 1995 *Interfaces in crystalline materials* (Clarendon Press)

[47] Yamakov V, Wolf D, Phillpot S R, Mukherjee A K and Gleiter H 2003 Deformation-mechanism map for nanocrystalline metals by molecular-dynamics simulation *Nat. Mater.* **3** 43–7

[48] Dao M, Lu L, Asaro R J, De Hosson J T M and Ma E 2007 Toward a quantitative understanding of mechanical behavior of nanocrystalline metals *Acta Mater.* **55** 4041–65

[49] Schiøtz J and Jacobsen K W 2003 A Maximum in the Strength of Nanocrystalline Copper *Science* **301** 1357–9

[50] Zhang K, Weertman J R and Eastman J A 2005 Rapid stress-driven grain coarsening in nanocrystalline Cu at ambient and cryogenic temperatures *Appl. Phys. Lett.* **87** 061921–061921 – 3

[51] Li C H, Edwards E ., Washburn J and Parker E . 1953 Stress-induced movement of crystal boundaries *Acta Metall.* **1** 223–9

[52] Van Swygenhoven H, Derlet P M and Hasnaoui A 2002 Atomic mechanism for dislocation emission from nanosized grain boundaries *Phys. Rev. B* **66** 024101

[53] Schiøtz J, Tolla F D D and Jacobsen K W 1998 Softening of nanocrystalline metals at very small grain sizes *Nature* **391** 561–3

[54] Aifantis K E and Ngan A H W 2007 Modeling dislocation—grain boundary interactions through gradient plasticity and nanoindentation *Mater. Sci. Eng. A* **459** 251–61

[55] Jin M, Minor A M, Stach E A and Morris Jr. J W 2004 Direct observation of deformation-induced grain growth during the nanoindentation of ultrafine-grained Al at room temperature *Acta Mater.* **52** 5381–7

[56] Sansoz F and Dupont V 2006 Grain growth behavior at absolute zero during nanocrystalline metal indentation *Appl. Phys. Lett.* **89** 111901–111901 – 3

[57] Sharon J A, Su P-C, Prinz F B and Hemker K J 2011 Stress-driven grain growth in nanocrystalline Pt thin films *Scr. Mater.* **64** 25–8

[58] Van Swygenhoven H and Derlet P M 2001 Grain-boundary sliding in nanocrystalline fcc metals *Phys. Rev. B* **64** 224105

[59] Badirujjaman S, Li X-W and Winning M 2007 Motion of [1 0 0]-tilt grain boundaries under cyclic stresses *Mater. Sci. Eng. A* **448** 242–8

[60] Legros M, Gianola D S and Hemker K J 2008 In situ TEM observations of fast grain-boundary motion in stressed nanocrystalline aluminum films *Acta Mater.* **56** 3380–93

[61] Bainbridge D W, Choh H L and H. Edwards E 1954 Recent observations on the motion of small angle dislocation boundaries *Acta Metall.* **2** 322–33

[62] Molodov D A, Gorkaya T and Gottstein G 2011 Dynamics of grain boundaries under applied mechanical stress *J. Mater. Sci.* **46** 4318–26

[63] Sansoz F and Molinari J F 2004 Incidence of atom shuffling on the shear and decohesion behavior of a symmetric tilt grain boundary in copper *Scr. Mater.* **50** 1283–8

[64] Janssens K G F, Olmsted D, Holm E A, Foiles S M, Plimpton S J and Derlet P M 2006 Computing the mobility of grain boundaries *Nat. Mater.* **5** 124–7

[65] Saldana C, Murthy T G, Shankar M R, Stach E A and Chandrasekar S 2009 Stabilizing nanostructured materials by coherent nanotwins and their grain boundary triple junction drag *Appl. Phys. Lett.* **94** 021910–021910 – 3

[66] Kumar K ., Van Swygenhoven H and Suresh S 2003 Mechanical behavior of nanocrystalline metals and alloys *Acta Mater.* **51** 5743–74

[67] Sanders P G, Eastman J A and Weertman J R 1997 Elastic and tensile behavior of nanocrystalline copper and palladium *Acta Mater.* **45** 4019–25

[68] Brooks I, Lin P, Palumbo G, Hibbard G D and Erb U 2008 Analysis of hardness–tensile strength relationships for electroformed nanocrystalline materials *Mater. Sci. Eng. A* **491** 412–9

[69] Czubayko U, Sursaeva V G, Gottstein G and Shvindlerman L S 1998 Influence of triple junctions on grain boundary motion *Acta Mater.* **46** 5863–71

[70] Mompiou F, Caillard D and Legros M 2009 Grain boundary shear–migration coupling—I. In situ TEM straining experiments in Al polycrystals *Acta Mater.* **57** 2198–209

[71] Valiev R 2004 Nanostructuring of metals by severe plastic deformation for advanced properties *Nat. Mater.* **3** 511–6

[72] Beyerlein I J, Lebensohn R A and Tomé C N 2003 Modeling texture and microstructural evolution in the equal channel angular extrusion process *Mater. Sci. Eng. A* **345** 122–38

[73] Kopylov V I and Chuvil'deev V N 2006 Ultimate Grain Refinement by ECAP: Experiment and Theory *Nanostructured Materials by High-Pressure Severe Plastic Deformation* NATO Science Series ed Y T Zhu and V Varyukhin (Springer Netherlands) pp 69–76

[74] Humphreys F J and Hatherly M 2012 *Recrystallization and Related Annealing Phenomena* (Elsevier)

[75] Doherty R D, Hughes D A, Humphreys F J, Jonas J J, Jensen D J, Kassner M E, King W E, McNelley T R, McQueen H J and Rollett A D 1997 Current issues in recrystallization: a review *Mater. Sci. Eng. A* **238** 219–74

[76] Rios P R, Siciliano Jr F, Sandim H R Z, Plaut R L and Padilha A F 2005 Nucleation and growth during recrystallization *Mater. Res.* **8** 225–38

[77] GOTTSTEIN G and MECKING H 1985 9 - Recrystallization *Preferred Orientation in Deformed Metal and Rocks* ed H-R Wenk (San Diego: Academic Press) pp 183–218

[78] Doherty R D, Hughes D A, Humphreys F J, Jonas J J, Juul Jensen D, Kassner M E, King W E, McNelley T R, McQueen H J and Rollett A D 1998 Current issues in recrystallization: A review *Mater. Today* **1** 14–5

[79] Urai J L, Means W D and Lister G S 1986 Dynamic Recrystallization of Minerals *Mineral and Rock Deformation: Laboratory Studies: The Paterson Volume* ed B E Hobbs and H C Heard (American Geophysical Union) pp 161–99

[80] Drury M R and Urai J L 1990 Deformation-related recrystallization processes *Tectonophysics* **172** 235–53

[81] Urai J L and Jessell M 2001 Recrystallization and grain growth in minerals: recent developments *Recrystallization and Grain Growth, Proceedings of the first joint international conference, Springer Verlag, in press. edited by G. gottstein and D Molodov*

[82] Galiyev A, Kaibyshev R and Gottstein G 2001 Correlation of plastic deformation and dynamic recrystallization in magnesium alloy ZK60 *Acta Mater.* **49** 1199–207

[83] Andrade U, Meyers M A, Vecchio K S and Chokshi A H 1994 Dynamic recrystallization in high-strain, high-strain-rate plastic deformation of copper *Acta Metall. Mater.* **42** 3183–95

[84] Luton M J and Sellars C M 1969 Dynamic recrystallization in nickel and nickel-iron alloys during high temperature deformation *Acta Metall.* **17** 1033–43

[85] Ardakani M G and Humphreys F J 1993 High Temperature Deformation and Dynamic Recrystallization of some Two-Phase Copper Alloys *Mater. Sci. Forum* **113-115** 213–8

[86] Palumbo G, Thorpe S J and Aust K T 1990 On the contribution of triple junctions to the structure and properties of nanocrystalline materials *Scr. Metall. Mater.* **24** 1347–50

[87] Klement U, Erb U, El-Sherik A M and Aust K T 1995 Thermal stability of nanocrystalline Ni *Mater. Sci. Eng. A* **203** 177–86

[88] King A H 1999 The Geometric and Thermodynamic Properties of Grain Boundary Junctions *Interface Sci.* **7** 251–71

[89] Gottstein G and Shvindlerman L S 2013 Grain boundary junctions, ridges and facets: their kinetics and effects on grain microstructure evolution *Emerg. Mater. Res.* **2** 71–8

[90] Mattissen D, Molodov D A, Shvindlerman L S and Gottstein G 2005 Drag effect of triple junctions on grain boundary and grain growth kinetics in aluminium *Acta Mater.* **53** 2049–57

[91] Gianola D S, Eberl C, Cheng X M and Hemker K J 2008 Stress-Driven Surface Topography Evolution in Nanocrystalline Al Thin Films *Adv. Mater.* **20** 303–8

[92] Gianola D S, Van Petegem S, Legros M, Brandstetter S, Van Swygenhoven H and Hemker K J 2006 Stress-assisted discontinuous grain growth and its effect on the deformation behavior of nanocrystalline aluminum thin films *Acta Mater.* **54** 2253–63

[93] Rupert T J, Gianola D S, Gan Y and Hemker K J 2009 Experimental Observations of Stress-Driven Grain Boundary Migration *Science* **326** 1686–90

[94] Merkle K L, Thompson L J and Phillipp F 2004 In-Situ HREM Studies of Grain Boundary Migration *Interface Sci.* **12** 277–92

[95] Dynkin N K and Gutkin M Y 2012 Migration of grain boundaries in free-standing nanocrystalline thin films *Scr. Mater.* **66** 73–6

[96] S.V. Bobylev I A O 2009 Mobility of Triple Junctions of Grain Boundaries during Their Migration in Deformed Nanocrystalline Materials *Rev. Adv. Mater. Sci.* **22** 39–51

[97] Darvishi Kamachali R and Steinbach I 2012 3-D phase-field simulation of grain growth: Topological analysis versus mean-field approximations *Acta Mater.* **60** 2719–28

[98] Krill III C E and Chen L-Q 2002 Computer simulation of 3-D grain growth using a phase-field model *Acta Mater.* **50** 3059–75

[99] Moelans N, Blanpain B and Wollants P 2008 Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems *Phys. Rev. B* **78** 024113

[100] Potts R B 1952 Some generalized order-disorder transformations *Math. Proc. Camb. Philos. Soc.* **48** 106–9

[101] Yu Q and Esche S K 2003 Three-dimensional grain growth modeling with a Monte Carlo algorithm *Mater. Lett.* **57** 4622–6

[102] Zöllner D 2011 A Potts model for junction limited grain growth *Comput. Mater. Sci.* **50** 2712–9

[103] Velasco M, Van Swygenhoven H and Brandl C 2011 Coupled grain boundary motion in a nanocrystalline grain boundary network *Scr. Mater.* **65** 151–4

[104] Gianola D S, Farkas D, Gamarra M and He M 2012 The role of confinement on stress-driven grain boundary motion in nanocrystalline aluminum thin films *J. Appl. Phys.* **112** 124313–124313 – 10

[105] Gottstein G and Shvindlerman L S 2005 Grain microstructure evolution and grain boundary junction engineering *Mater. Sci. Technol.* **21** 1261–6

[106] Chellali M R, Balogh Z, Bouchikhaoui H, Schlesiger R, Stender P, Zheng L and Schmitz G 2012 Triple Junction Transport and the Impact of Grain Boundary Width in Nanocrystalline Cu *Nano Lett.* **12** 3448–54

[107] Allen M P 2004 Introduction to molecular dynamics simulation *Comput. Soft Matter Synth. Polym. Proteins* **23** 1–28

[108] Anon Kochmann Research Group - California Institute of Technology

[109] Daw M S and Baskes M I 1984 Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals *Phys. Rev. B* **29** 6443–53

[110] Frenkel D and Smit B 2002 *Understanding Molecular Simulation: From Algorithms to Applications* (Academic Press)

[111] Tsai D H 1979 The virial theorem and stress calculation in molecular dynamics *J. Chem. Phys.* **70** 1375–82

[112] Plimpton S 1995 Fast Parallel Algorithms for Short-Range Molecular Dynamics *J. Comput. Phys.* **117** 1–19

[113] Mishin Y, Mehl M J, Papaconstantopoulos D A, Voter A F and Kress J D 2001 Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations *Phys. Rev. B* **63** 224106

[114] Grochola G, Russo S P and Snook I K 2005 On fitting a gold embedded atom method potential using the force matching method *J. Chem. Phys.* **123** 204719

[115] Mendelev M I, Kramer M J, Hao S G, Ho K M and Wang C Z 2012 Development of interatomic potentials appropriate for simulation of liquid and glass properties of NiZr2 alloy *Philos. Mag.* **92** 4454–69

[116] Mendelev M I, Kramer M J, Becker C A and Asta M 2008 Analysis of semi-empirical interatomic potentials appropriate for simulation of crystalline and liquid Al and Cu *Philos. Mag.* **88** 1723–50

[117] Williams P L, Mishin Y and Hamilton J C 2006 An embedded-atom potential for the Cu–Ag system *Model. Simul. Mater. Sci. Eng.* **14** 817

[118] Nosé S 1984 A unified formulation of the constant temperature molecular dynamics methods *J. Chem. Phys.* **81** 511–9

[119] Hoover W G 1985 Canonical dynamics: Equilibrium phase-space distributions *Phys. Rev. A* **31** 1695–7

[120] Li J 2003 AtomEye: an efficient atomistic configuration viewer *Model. Simul. Mater. Sci. Eng.* **11** 173

[121] Faken D and Jónsson H 1994 Systematic analysis of local atomic structure combined with 3D computer graphics *Comput. Mater. Sci.* **2** 279–86

[122] Aramfard M and Deng C 2014 Influences of triple junctions on stress-assisted grain boundary motion in nanocrystalline materials *Model. Simul. Mater. Sci. Eng.* **22** 055012

[123] Upmanyu M, Smith R W and Srolovitz D J 1998 Atomistic Simulation of Curvature Driven Grain Boundary Migration *Interface Sci.* **6** 41–58

[124] Bernstein N 2008 The influence of geometry on grain boundary motion and rotation *Acta Mater.* **56** 1106–13

[125] Ovid'ko I A, Sheinerman A G and Aifantis E C 2008 Stress-driven migration of grain boundaries and fracture processes in nanocrystalline ceramics and metals *Acta Mater.* **56** 2718–27

[126] Gutkin M Y and Ovid'ko I A 2005 Grain boundary migration as rotational deformation mode in nanocrystalline materials *Appl. Phys. Lett.* **87** 251916

[127] Rybin V V, Zisman A A and Zolotorevsky N Y 1993 Junction disclinations in plastically deformed crystals *Acta Metall. Mater.* **41** 2211–7

[128] Rybin V and Zhukovskii I 1978 Disclination mechanism of microcrack formation *Sov Phys Solid State* **20** 1056–9

[129] Rybin V and Zisman A 1985 Contact disclinations in plastically deformed crystals. *SOV PHYS SOL ST* **27** 105–10

[130] Nazarov A A 2013 Disclinations in bulk nanostructured materials: their origin, relaxation and role in material properties *Adv. Nat. Sci. Nanosci. Nanotechnol.* **4** 033002

[131] Sakai T, Belyakov A, Kaibyshev R, Miura H and Jonas J J 2014 Dynamic and post-dynamic recrystallization under hot, cold and severe plastic deformation conditions *Prog. Mater. Sci.* **60** 130–207

[132] Armstrong R W 1968 Wedge dislocation as the elastic counterpart of a crystal deformation twin *Science* **162** 799–800

[133] Wu X L, Liao X Z, Srinivasan S G, Zhou F, Lavernia E J, Valiev R Z and Zhu Y T 2008 New Deformation Twinning Mechanism Generates Zero Macroscopic Strain in Nanocrystalline Metals *Phys. Rev. Lett.* **100** 095701

[134] Drury M R and Humphreys F J 1986 The development of microstructure in Al-5% Mg during high temperature deformation *Acta Metall.* **34** 2259–71

[135] Miura H, Sakai T, Mogawa R and Jonas J J 2007 Nucleation of dynamic recrystallization and variant selection in copper bicrystals *Philos. Mag.* **87** 4197–209

[136] Poliak E I and Jonas J J 1996 A one-parameter approach to determining the critical conditions for the initiation of dynamic recrystallization *Acta Mater.* **44** 127–36