NEW DISCRETE DISLOCATION ALGORITHMS IN PLASTIC DEFORMATION AND ITS APPLICATION TO RATE EFFECT, CREEP AND FRACTURE

A Dissertation Presented

By

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to

The Department of Mechanical and Industrial Engineering

in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

in the field of

Mechanical Engineering

Northeastern University
Boston, Massachusetts

August 2016
ABSTRACT

Given that thermal activation and climb of dislocation contribute significantly to high temperature plastic behavior, creep and fracture, a thorough understanding of dislocation motion is extremely critical. A new discrete dislocation model is presented to solve the three: (i) the time scale gap between dislocation glide and other thermal process, (ii) plastic deformation when dislocation lines are thermally activated over an obstacle field and (iii) dislocation climb due to the vacancy diffusion at a wide range of time scale.

The first problem occurs when current Discrete Dislocation Dynamics model wants to reach experiment-level of strain rate or time scale while keeps tracking the dislocation glide at very small time step. The essential idea is to avoid tracking the dislocation path, instead using energy minimization to determine the equilibrium configuration under given boundary conditions. In our model all other processes exclusive to glide - short range effects, thermally activated escape and dislocation climb - that change the energy of the system are modeled as discrete events which are defined by constitutive rules or by solving an auxiliary diffusion boundary value problem. This approach allows decoupling of time scales associated with dislocation glide and it enables modeling both rate and temperature effects of interest in practical applications.

The second problem arises when overall plastic behavior is controlled by the local dislocation-obstacle interaction at finite temperature. For a system in which the strain
energy is minimized, dislocations are either in equilibrium or pinned against obstacles. Thermal activation can now be incorporated using a general energy model and an average waiting time. The deterministic two-dimensional thermal escape model can thus be viewed as a statistical average of the three-dimensional stochastic process. This strategy is independent of the obstacle energy model and hence a variety of strengthening mechanism can be employed. The numerical results displays positive rate sensitivity for one energy model and the computational cost among different strain rate remains the same order.

The third problem is very significant to creep. For the auxiliary diffusion problem that enables dislocation climb, most of the study is confined to steady state and the missing part is the transient to steady state as a function of applied load and microstructure. Therefore, a universal dislocation model is presented. Three innovative points are (a) computing the rate of climb of dislocations at arbitrary temporal scales, (b) coupling of vacancy concentration fields between dislocations that are close together and (c) solving a coupled mechanical-diffusion problem accurately. Further cases show that at different temperature and strain rate, a competition between thermal activation and climb occurs, resulting in different material strength.

In summary, the proposed model captures the three basic motion of dislocation: glide, climb and thermal activation. It breaks the current computation limit and provides a new outlook in examining the creep, fracture and fatigue in large temporal scale.
ACKNOWLEDGEMENT

The past five years has been the longest time so far that I devoted myself into a challenging scientific problem. Although I am satisfied my accomplishment, the pursuit of the Ph.D. degree is a tough journey. Finally I pushed myself to the limit to make it through. However, this research cannot be completed without the support of people around. I would like to express my gratitude to all of them.

The most two important people in the past years would be my adviser, Srinath Chakravarthy and my girl friend, Yan Xiaofeng. Srinath is a knowledgeable and enthusiastic young scholar who join Northeastern University at the same year as I did. Together we build the research platform from scratch and for the first three years he fight beside me in the front line. Discussion, debugging and improving goes on day by day until I can work dependently. Meanwhile, Xiaofeng and I maintains a relationship that is 6000 miles in space and 12 hours in time. She is the best girl that I have ever, never met in this world and the future life of us has always motivated me moving forward. There used to be a major emotional crisis during the middle of one semester. During that hard time, I felt desperately going back the save our love but a very important conference is ahead. Srinath and his family provide a huge support that they encourage me go back and talk to her in person. That was a very important time in my life. Otherwise, I might have lost my girl.

I own my parents a lot. They are always concern with me. However, I talk to them less and less frequently due to the pressure. They may not be able the understand
my research but they always encourage me to be strong and persistent. To them, I only have a simple word that they can read: I love you both.

In the Northeastern University, I come across with a lot of excellent people. My committee members, Sinan Müftü and Monnesh Upmanyu, help me to establish a thorough understanding in mechanics and diffusion, which boost my research and enrich my philosophy of life as well. Also, I would thank Professor George G. Adams, Kai-Tak Wan and Miriam Leeser for the academic advise. James Martino, a talented and easy-going man in my group and Upmanyu’s group members. It is a awesome experience working and studying with them.

I would also thank my current and former roommates: Zhao Qian, Yin Fei, Li Yi, Lin Yichun, Sun Qian, Hao Ji and Qiao Ju. We have a lot of good time together. Some of them have gone back to China and I look forward to meet them again. Besides, I would thank my classmates Pu Yu, Yang Hankang and Song Kenan.

Finally, this work is in memory of my friend, Lin Jingyuan, who past away in April 2012 due to a very rare cancer. He and I are only two Chinese Ph.D. students who admitted by Department of Mechanical Engineering in Fall 2011. Unfortunately, he could never finish his study. Therefore, I would like share my work with him and let Northeastern remember such a a good young man. May he rest in peace in heaven and I would send my best regards to his family for the great loss.
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CHAPTER 1

INTRODUCTION

The material structure and its relation with the materials properties is an importu-
nate aspect of material science research, which provides guidance in designing the
new materials. Therefore, the iterative study on structure, property and performance
expands the knowledge to the material in both spatial and temporal scale. With the
emergence of large-scale computational capabilities and the advance of experimental
techniques, people aimed to establish more precise models to incorporate known
mechanisms with less calibration parameters. Meanwhile, compared with empirical
top-down model, the mechanism-based bottom-up model provides more fundamental
understanding to material behavior and lower the cost in discovering new materials.
This research is focused on modeling the micro plasticity in the crystalline material.

1.1 From continuum to discreteness

In macroscale, the plastic deformation is viewed as 'flow'. The conventional plasticity
theory gives a nice description by the yielding criteria and flow rule, which has a good
agreement with the experiments. However, as the sample size becomes smaller, the
plastic behavior deviates from that of the bulk material. This size dependency has
been observed in indentation [2], micropillar compression [3], bending [4], thin film
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[5] and fatigue [6]. A review can be found in [7]. One interpretation of the size effects is triggered by the multiplication and storage of dislocation and its interaction with other defect of the crystal.

Dislocation is a type of line defect within the crystalline material. Dislocations can be created by shearing a perfect crystal when a bond is broken and form a new bond with adjacent atom. Therefore, an extra half plane of atom is generated with crystal. The magnitude and direction of the dislocation can be characterized by Burgers vector. An important feature of dislocation is that it can glide or climb within the crystal, making it the main carrier of the plastic deformation. So, when the sample size is going smaller, the discreteness of the dislocation begins to merge. When going down to micro or nanoscale, the plastic strength is strongly depending on the discreteness and randomness of material structure, such as dislocation-dislocation, dislocation-obstacle and dislocation-crack tip interaction. This can not be captured by conventional plasticity theory. Therefore, it gives rise to the strain/stress gradient plasticity and the discrete dislocation dynamics (DDD).

1.1.1 Gradient plasticity theory

Strain gradient plasticity is the first continuum theory that attempts to capture the size effect. A review of strain gradient plasticity can be found in [8]. The general idea is that besides the strain tensor, the gradient of strain tensor is also introduced into the constitutive law and an inner 'length' is automatically associated with gradient. This inner length makes strain gradient plasticity accounts for the size effect. Although different theories have different physical explanations of the 'inner length', strain gradient theory has shown its capabilities in capturing the size effect. New progress has been made in recent years. Gurtin [9] introduces a small-strain strain gradient theory which is thermodynamically feasible. Wei et al. [10] applies strain gradient plasticity to the crack growth problem. Also the non-convex rate dependent strain
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Gradient crystal plasticity [11] and the fully coupled glide-climb strain gradient crystal plasticity model [12] is developed.

Another attempt is the stress gradient theory [13] which uses the gradient of elastic stress tensor as new parameter to the plastic model. The advantage of stress gradient theory is that it has clear physical length associated with stress gradient. So far, the strain gradient has been applied to in crack propagation [14] and its framework is not fully developed.

1.1.2 Discrete dislocation dynamics

Discrete dislocation dynamics (DDD) is a computational model that solves a continuum linear elastic problem that contains a number of individual dislocations. Each dislocations is treated as a movable entity with long range elastic stress field. To account for the dislocation multiplication and storage, DDD also defines a set of constitutive laws for short range effects, such as dislocation nucleation, dipole annihilation, pinned dislocations escaping from obstacles without thermal assistance and dislocations absorbed by the boundary. The input of DDD is the sample geometry, mechanical boundary conditions, elastic material properties, Burgers vector, slip system and obstacle/source. The output of DDD is plastic deformation and dislocation pattern. First, planar DDD framework was developed, followed by the full three dimensional DDD.

Two dimensional discrete dislocation dynamics (2d DDD) Two dimensional discrete dislocation dynamics is developed to solve the two dimensional elastic problem with edge dislocation (dislocation that its Burgers vector and dislocation line are perpendicular to each other). In 2d DDD, dislocation line is perpendicular out of the plane so that dislocation is projected as a point to the problem plane. The
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elastic boundary value problem (BVP) is solved based on the superposition principal. Lubarda et al. [15] studied the equilibrium pattern of dislocation by minimizing potential energy. Van der Giessen and Neeleman [16] established the superposition framework from the principle of virtual work. These two papers set up the basic methodology of 2d DDD. Later 2d DDD is extended to non-convex domain [17] where the displacement field of the step created in the inner surface is treated correctly. Also, a framework that solve a finite strain problem is also proposed [18].

The plastic deformation comes from the glide of a large number of dislocations. In DDD, the dislocation glide follows Newton’s second law (1.1) with the applied force $b\sigma$ on the dislocation

$$M\ddot{x} + B\dot{x} = b\sigma$$

where $x$ is local coordinate, $b$ is magnitude of Burgers vector, $M$ is mass per unit length, $B$ is drag coefficient and $\sigma$ is applied stress. Equation (1.1) reflects that the inertial force $M\ddot{x}$ and the drag force $B\dot{x}$ is balanced by driving force $b\sigma$. Here a quasi-state assumption is made such that the inertia effect is neglected. This assumption holds true except in very fast loading case. Hence the dislocation velocity $v = \dot{x}$ under driving force $F = b\sigma$ is written as

$$v = \frac{F}{B}$$

(1.2)

Considering the speed of dislocation and problem size, the time step to capture the dislocation motion is $10^{-11} \sim 10^{-10}$ s. That defines a time scale associated with dislocation glide.

The two-dimensional plane-strain DDD has been used to provide fundamental insight into a variety of problems including fatigue crack growth in single crystals [19] and polycrystals [20], crack growth in thin films [21], confined layers Keralavarma and Benzerga [22], bi-material interfaces [23], and size effects in deformation [24] and
1.1. FROM CONTINUUM TO DISCRETENESS

fracture [13]. Studies incorporating strain rate effects, temperature - and consequently climb and thermal activation of dislocations over obstacles - have been extensively studied [25, 26, 27, 28, 29]. But relatively few DDD simulations have incorporated these effects [30].

Three dimensional discrete dislocation dynamics (3d DDD) Three dimensional discrete dislocation dynamics [31] is able to naturally reproduce Frank-Read nucleation, the cross-slip, the dislocation junction formation or the multiple slip configuration, in spite of its computational expense. The main feature is that the dislocation loop is modeled as piece-wise straight segment consisting by nodes. Also, the finite body boundary is more complicated than 2d DDD [32].

So far 3d DDD models have led to significant insight into strain hardening due to forest dislocation interactions Madec et al. [33], Madec [34], Chen et al. [35], Kubin et al. [36], Alankar et al. [37], deformation of nano-scale pillars Weygand et al. [38], Akarapu et al. [39] and beams [40], and individual dislocation crack tip interactions [41]. However, their application has been limited due to high computational cost [42]. Also for many alloyed materials, capturing both local dislocation-obstacle interactions and larger scale dislocation-dislocation interactions simultaneously is a challenge in 3d.

1.1.3 Summary

From continuum to discreteness, the impact of the substructure evolution begins to merge. To capture to size effect, the gradient plasticity theory and discrete dislocation dynamics shows two different ways of thinking. The gradient plasticity theory as a natural extension to phenomenological method, is a top-down model that links the macroscale. It takes advantage of concise format, easy to incorporate with finite element method (FEM) and less computation. On the other hand, discrete dislocation
1.2. THERMAL ACTIVATION AND RATE SENSITIVITY

Dynamics is a bottom-up model which has less prerequisites in the exchange of more computational cost. It enables to reproduce substructure evolution. Therefore DDD provides more fundamental understanding of the material strengthening and mechanism. Also it could play as an inter-connector to the macroscale above and nanoscale below. Over decades of development, discrete dislocation dynamics is a mature field. The goal of our research is extending the DDD tool to solve more general problem. In the discussion above, we have emphasized how the DDD evolved to accommodate the length scale changes. In the following section, we will go through the work that incorporating DDD with different time scale, thermal activation and diffusive climb receptively.

1.2 Thermal activation and rate sensitivity

All the strengthening mechanism work by impeding dislocation glide. In DDD, the distributed obstacle within the body is main part prohibiting dislocation motion. The obstacle model in original DDD is quite simple. When the force on the pinned dislocation is greater than the obstacle strength, the dislocation is released from that obstacle and keeps moving. We may potentially replace obstacle model to mimic variety of strengthening mechanism. This section will focus on thermal activation over obstacle and its impact on the property.

1.2.1 Athermal model of obstacle

The athermal theoretical models aim to establish the critical resolved shear stress (CRSS) for dislocation lines cross over obstacle fields as functions of the obstacle distribution, obstacle strength and applied shear stress. There are two main categories of the obstacle model. Friedel model [43, 44] is for high obstacle strength, but low obstacle density along the dislocation line, where the obstacles only provide resistance
force. This model is used in precipitation strengthening [45]. Labush model [46, 47] is for weak obstacle but high obstacle density, where interaction between the dislocation line and obstacle may be assisting or resisting the motion. Dislocation bypasses the entire set of obstacles and remain almost straight afterward. This model is used in solid-solution strengthening.

In terms of simulation, the obstacle could represent variety of material structures such as solute atom, precipitate phase or grain boundary. Therefore the obstacle parameters should be general enough and independent of dislocation configuration. Hence we will introduced the concept of 'stress equivalence', which is first proposed by Bansinki [48] that solution hardening is stress equivalent, not directly depending on the concentration of the solute. Then Argon [27] reiterated stress equivalence as the average resistance over the coherent length and provided a thermal activation format, where the coherent length [49] is defined such that when dislocation line cross one pinning point, another is met.

### 1.2.2 Thermal activation in DDD

The thermal activation process is stochastic process along the dislocation line. It can only be done on average. Frank [50] found that when dislocations glide through an obstacle spectrum with different energy barrier, the slip rate flows the Arrhenius equation with mean free energy of activation. Then Kocks et al. [25] presented the empirical law to account for variety of mechanisms.

The thermal activation in DDD is usually performed on single slip plane and different factors are considered. Early work has characterized the the point obstacle or continuous obstacle with free energy barrier [51] and established an average escaping frequency as a function of obstacle field parameters [52]. Mohles et al. [53] found that the thermal activation over an obstacle field can well be compared to an obstacle spectrum with constant spacing and can be further simplified to a continuous obstacle
1.2. THERMAL ACTIVATION AND RATE SENSITIVITY

Wall. Hiratani and Nadgorny [26] developed a computational model about dislocation glide through distributed obstacles by thermal activation. The dislocation motion is decoupled into three parts: thermally activation from the equilibrium position at the obstacle, running time to the next obstacle and dynamics transient to the next equilibrium position. Based on this decomposition, the competition between running time by dislocation inertia and waiting time by thermal activation is investigated and the results agree with experiment. Picu et al. [28] studied the thermally activated dislocation motion bypassing the field with two different types of obstacle. They found that dislocation motion undergoes a transition from smooth unzipping mode to jerky mode which is controlled by a threshold stress. In each regime, the strain rate sensitivity is governed by different parameters. Monnet et al. [29] showed that the thermal activation over obstacle field is depending on the screw part of dislocation segment as well where the effects can be characterized by an effective length. Dong et al. [54] showed that flow stresses due to different obstacle strengthening mechanisms are additive only when all strengthening obstacles can be approximated as point-like obstacles. When the activation distance of the low-density obstacles exceeds the spacing between the high-density obstacles, the flow stress is non-additive. However, all the models mentioned above are only performed on the single slip plane but not with multiple slip plane or slip system.

1.2.3 Summary

Therefore, with the extensive studies on the rate effects in single slip plane, the missing part is how these models interact with a whole dislocation configuration and what the collective responds to the strength is. Currently the coupling between thermal activation with tension, bending and crack has not been examined yet [30]. The main reason is that it is hard to find an equilibrium configuration in the framework of DDD. Besides, since thermal activation is rate sensitive and time scale is constrained by the
dislocation glide, performing large-scale DDD for low strain rate is very computationally costly.

1.3 Dislocation climb

Besides the thermal activation, diffusion-assisted climb has another time scale that DDD has to accommodate. Dislocation could form jogs along the dislocation line by vacancy diffusion towards the core and eventually jump to the next atom plane. This process typically happens much slower than dislocation glide depending on the temperature. The vacancy transportation in the bulk is governed by the diffusion equation. The boundary condition is defined on the inner surface around each dislocation which a radius of a few manometers, whereas the sample size is in microns or larger. Therefore the direct meshing and solving the diffusion BVP that contains large numbers of dislocations by finite element method is actually intractable. A semi-analytic method is often used in solving this coupled BVP where dislocations is replaced as point source/sink. We will first review the development of dislocation climb BVP and then discuss the incorporation with DDD.

1.3.1 Continuum and mesoscale model

The transient problem of dislocation climb can be treated as a continuous source with constant concentration in the core region. The general expression of concentration profile and flux in cylindrical coordinate is singular a integral [55, 56]. A series of attempts [57, 58, 59, 60, 61] were made to approximate the flux. Perrochet [60] gave a concise close form approximation with very good accuracy.

Ham [62] firstly described time-dependent diffusion-limited precipitation, which gives the particle concentration and the particle radius growth as a function of time. Ballufi and Seidman [63, 64] gives the climb rate of straight dislocation in diffusion
1.3. DISLOCATION CLIMB

limited case. They point out that in diffusion limited case, dislocation motion is not a
significant factor affecting the climb rate. Also the transient solution can be replaced
by a steady-state solution by assuming that the concentration at the boundary is equal
to the mean concentration within the control volume. This approach is adopted to
3d discrete dislocation dynamics by Mordehai [65] where dislocation is considered as
a perfect source/sink, corresponding to diffusion limited case.

Bakó and Hoffelner [66] provide coarse grain model to examine cellular pattern
formed by preexisting dislocations with and without externally loads. The climb is
introduced by drag law similar with (1.2), where the drag coefficient is 1000 times
smaller than that of the glide.

Gao and Cocks [67] give a general framework for dislocation climb based on ther-
modynamics variational approach within diffusion limited region. The BVP is set up
and the driving force is given in the forms of a chemical potential. Based on this
work, a fully coupled glide-climb strain gradient crystal plasticity model is developed
[12].

In polycrystalline, Lebensohn et al. [68] presents continuum constitutive law that
incorporates dislocation glide and climb. The creep behavior is studied at high tem-
perature and low strain rate.

1.3.2 Climb in discrete dislocation dynamics

The climb is introduced to DDD in mainly two different ways. In one the climb rate
is directly given by a drag law similar to (1.1) without solving the vacancy diffusion
BVP. Raabe [69] provides a framework of incorporating non-conservative motion into
3d discrete dislocation dynamics. The climb motion is governed by the Newton’s law
of motion where the driving force with a time scale of $10^{-12} \sim 10^{-11}$s. A follow-up to
this work is the grain boundary motion by combining conventional 2d DDD with bulk
diffusion [70]. In order to accommodate the time scale between dislocation glide and
1.3. DISLOCATION CLIMB

diffusion, they apply high temperature high rate to accelerate the simulation speed. Also, the drag law climb is used in cellular pattern study [66], the polycrystalline thin film [71], the finite strain problem [72] and the creep of Nickel based superalloys [73].

The other ways is by solving the diffusion, static or transient, to obtain the climb rate. Mordehai et al. [65] established a framework that combine diffusion-controlled dislocation climb with 3d DDD. The climb rate is calculated under the steady state assumption in the vicinity of the dislocation line in the case that the dislocation glide is prohibited. Gao et al. [74] investigate the role of pipe diffusion in 3d DDD framework where pipe diffusion is assumed to be independent of bulk diffusion and steady state. Po and Ghoniem [75] established a variational framework that coupled mechanical, temperature and vacancy concentration field in 3d DDD under steady state case. Two constraints are considered and implemented: one is the thermal dissipation, the other is the conservation of vacancy over a control volume which gives the climbing velocity. Another recent work [76] considers the concentration coupling between two discoloration loops in 3d, showing that dislocation climb rate is also depending the dislocation pattern. The framework is also steady state. In 2d DDD, the power law relation between strain rate and flow stress is studied [77] where the glide and climb time scales are manually decoupled by a adjustable time step scheme. Later another 2d DDD framework [1] is presented. Here the local diffusion of vacancy around dislocation core is no longer assumed as steady state but time dependent by superposing a series of instantaneous point sources. A superposition on diffusion BVP similar to DDD is used to remove the computation difficulty in direct meshing. However this framework is still computational expensive and it only operate on the time scales that comparable with glide.

The efficiency of inner interface around the dislocation is also considered [78]. The climb rate is controlled by bulk diffusivity when dislocation operates as perfect source/sink, corresponding to a diffusion limited case. By introducing the efficiency
of the source/sink, climb rate is determined by kinetics across the interface, corresponding to source-limited case. The diffusion limited case and source limited case by is incorporated with 2d DDD [1, 72].

1.3.3 Summary

To accommodate the difference between the glide and climb time scales, people use different drag coefficient [66, 71, 72, 73], or scaling time or diffusion coefficient [70, 1], or combination of local steady/quasi-steady state solution with global transient solution [65, 74, 77]. All these trade-off is to maintain a reasonable simulation time.

1.4 Application of discrete dislocation dynamics

Since DDD has successfully captured the plastic deformation at micron scales, it has been applied to variety of problems.

1.4.1 Crack growth

The continuum frame for fracture mechanics has been well established. In interaction between crack tip and dislocation is controlled by the three types of energies: crack tip toughness [79, 80], stress field and dislocation shielding of the crack tip [81] and dislocation emission from the crack tip [82, 83].

Cleveringa et al. [19] first propose a framework of crack growth in 2d DDD. A boundary value problem with cohesive zone is given. A half space solution of a dislocation is used to ensure the traction free surface on the left. The effect of source and obstacle density on the crack growth, which is characterized by the tip advance and normalized stress concentration, is discussed. Later a rate sensitivity study [84], and fatigue simulation [85] are performed.
1.4. APPLICATION OF DISCRETE DISLOCATION DYNAMICS

O’day and Curtin [23, 86] establish a new superposition framework for 2d DDD and apply it to crack growth and bi-material interface. All the dislocations are wrapped up in a DDD sub-problem which enables flexibility when dealing with the cohesive boundary conditions.

Chakravarthy and Curtin [21] carry out 2d DDD simulation for crack propagation and identify that obstacle spacing the govern the fracture toughness. This conclusion is then generalized as “stress gradient plasticity” [13].

1.4.2 Nickel-based superalloys

Nickel-based $\gamma/\gamma'$ superalloys are extensively used in applications requiring high strength and fatigue resistance at elevated temperatures. Eggeler and Dlouby [87] carry out high temperature low stress creep experiment.

Vattre et al. (2009) [88] examine the flow stress for high volume fraction (up to 73%) Nickel-based $\gamma/\gamma'$ superalloys using 3d DDD. The influence of material composition and micro-structure parameter on the flow stress is discussed. The dislocation climb is not considered.

Haghighat et al. [73] investigate the creep behavior of Nickel based superalloys under 3d DDD.

1.4.3 Polycrystalline

The performance of polycrystalline material in homologous temperature is another important subject, which involve the diffusion along the grain boundary and grain boundary migration. Ahmed and Hartmaier [89] study the relationship between grain size and strength of the material using 2d DDD. They start with pre-existing dislocations and the Hall-Petch relation is recovered. However dislocation climb and
boundary motion is not considered. Later grain boundary motion \cite{70} is studied by combining conventional 2d DDD with bulk diffusion.

Davoudi et al.\cite{71} combine dislocation glide and climb within 2d DDD, where climb rate is calculated by drag law.

Quek et al.\cite{90} combine 2d DDD with grain boundary sliding and the absorption, emission and transmission of bulk dislocation at grain boundary.

1.5 Challenge and dissertation outline

We briefly review the discrete dislocation dynamics and its application in modeling micro-scale plasticity. Although DDD is a powerful tool to reproduce the evolution of micro-structure, it has much potential of improvement.

The main challenge of discrete dislocation dynamics is that its coherent glide time scale would generate computational difficulty when incorporated with other physical time scales. For example, to reach the desired strain within a reasonable simulation time, DDD usually use strain rate ($10^3 \text{s}^{-1}$) much higher than that of experiments($10^{-5} \sim 10^{-3} \text{s}^{-1}$). In athermal case, this makes no difference on material strength. However, under finite temperature, dislocations may be thermally activated over obstacles and thus material strength becomes quite sensitive to strain rate. This means that one should use actual strain rate otherwise the result may not reflect the actual physics. Another example is that combining dislocation climb with glide. Dislocation may climb to next slip plane by emitting or absorbing vacancies. However, vacancy diffusion defines time scales ($10^0 \sim 10^{-3} \text{s}$) much longer than the glide time scale ($10^{-11} \sim 10^{-10} \text{s}$). In either case, the straightforward simulation will become very expensive. This calls for new ways of modeling dislocation motion to fit the gap between different time scales.
From above we can see to maintain a reasonable computation time when dealing with thermal process in DDD, some trade-off technique are used. First, the configuration needs to be relaxed for period time to reach quasi-equilibrium state under applied load [66, 77]. Second, the simulation is performed in relatively high strain rate ($\sim 10^3 \text{s}^{-1}$) [71]. Third, in order to coordinate the different time scales between dislocation glide and climb, neither a artificial mobility ratio is introduced [66, 72, 73] nor a scaled time is used [1]. In order to avoid these artificial techniques, the quasi-static approximation is made such that the motion of a moving dislocation is accomplished instantaneously compared with thermal process when the boundary condition changes.

The goal of this research is to find a new way to model dislocation motion, enabling decoupled dislocation glide with other physical process in order to achieve long time scale. The rest of the dissertation is organized as follows. Chapter 2 solves the temporal scale challenge by coming up with a new energy minimization strategy to determine dislocation glide position at arbitrary time scales. Chapter 3 deals with the stochastic thermal activation with a general energy model which is applicable to a variety of microstructures. Chapter 4 models the dislocation climb at finite temperature and present a new analytical model for evaluating transient climb rates. Chapter 5 summarizes the main conclusions and propose the future research.
CHAPTER 2

DISLOCATION POSITION AT ARBITRARY TIME SCALE

The velocity of dislocation glide depends on the applied shear stress, purity of crystal, temperature and type of dislocation. The glide velocity range where drag law (1.2) applies is about 0.1 to 1000 m/s. Considering the average free path of dislocation is 1 nm to 1 µm depending on the crystal structure, the time scale to accurately capture dislocation motion is then chosen as $10^{-11}$ to $10^{-10}$ s [16]. However this glide time scale prevents DDD from long term simulation. So our first problem is to determine dislocation glide at an arbitrary time scale. The fundamental assumption in our model is that dislocation glide occurs on time scales that are much shorter than any other phenomena, such as dislocation nucleation, escape from obstacles and dislocation climb. The essential idea is to avoid tracking the dislocation path, instead using energy minimization to determine the equilibrium configuration under given boundary conditions, thereby eliminating the glissle time scale and allowing incorporation of thermally assisted events at the realistic time scales.
2.1 Formulation

For a given starting dislocation distribution and applied load, a constrained minimization of the strain energy results in a configuration where all dislocations are in equilibrium or pinned against point obstacles on their respective glide planes. A good example to illustrate the concept of energy minimization is dislocation pile-up, shown in Fig. 2.1. The leading dislocation is pinned at the obstacle while another free dislocation with the same sign moves towards it under a given external load. Eventually the free dislocation will reach a position where its net force equals zero, corresponding to a minimum in the strain energy.

The same process can be achieved by a strain energy minimization, without introducing the glide time or dislocation velocity. Consider \( n \) dislocations represented by an initial position \( s_i \) on a slip plane, with an obstacle at position \( s_{\text{obs}} \) preventing glide. Assume that \( s_1 < s_2 < \cdots < s_i < \cdots s_n < s_{\text{obs}} \) and each dislocation undergoes a change in position from \( s_i \) to \( s_i + \Delta s_i \) due to the externally applied load.
load. The change in the strain energy of the \(i^{th}\) dislocation \(\Delta E_i\) is then the sum of pairwise dislocation interaction energy \(\Delta E_{ij}^{\text{int}}\) (between dislocation \(i\) and \(j\)) and the work done by the external load in moving the dislocation \(\Delta E_i^{\text{ext}}\), such that

\[
\Delta E_i = \sum_{j=1, i \neq j}^{n} \Delta E_{ij}^{\text{int}} (\Delta s_i, \Delta s_j) + \Delta E_i^{\text{ext}} (\Delta s_i).
\]

Therefore, the change in the total strain energy of the system \(\Delta E = \sum_{i=1}^{n} \Delta E_i\). Thus, the problem can be formulated as finding the differential displacement \(\Delta s_i\) of the dislocations such that the total strain energy is minimized. In this context, the minimization of the total strain energy can be expressed by the following the optimization model

\[
\text{find } \Delta s = [\Delta s_1, \ldots, \Delta s_n] \quad \text{(2.1a)}
\]

\[
\min \Delta E = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1, i \neq j}^{n} \Delta E_{ij}^{\text{int}} (\Delta s_i, \Delta s_j) + \sum_{i=1}^{n} \Delta E_i^{\text{ext}} (\Delta s_i) \quad \text{(2.1b)}
\]

\[
\text{s.t. } s_1 + \Delta s_1 \leq \cdots \leq s_i + \Delta s_i \cdots \leq s_n + \Delta s_n \leq s_{\text{obs}} \quad \text{(2.1c)}
\]

where (2.1c) represents constraints on dislocation motion ensuring that two dislocations cannot pass each other or an obstacle.

An early work is [15]. The energy term \(\Delta E_{ij}^{\text{int}}\) and \(\Delta E_i^{\text{ext}}\) is obtained by integrating the glide component of Peach-Koehler force (2.2)

\[
F = (b \cdot \sigma) \times \xi \quad \text{(2.2)}
\]

where \(b\) is the Burgers vector of the dislocation, \(\xi\) is the unit vector tangent to the dislocation line, which points out of the paper and \(\sigma\) is the local elastic stress field of the other dislocation. To avoid the singularity of the dislocation core regions where linear elastic theory no longer apply, a non-singular continuum theory of dislocations Cai et al. [91] is used.
\[ \sigma_{xx} = -Ab \frac{y}{\rho_a^2} \left[ 1 + \frac{2 (x^2 + a^2)}{\rho_a^2} \right] \] (2.3a)

\[ \sigma_{yy} = Ab \frac{y}{\rho_a^2} \left[ 1 - \frac{2 (y^2 + a^2)}{\rho_a^2} \right] \] (2.3b)

\[ \sigma_{xy} = Ab \frac{x}{\rho_a^2} \left[ 1 - \frac{2y^2}{\rho_a^2} \right] \] (2.3c)

where \( A = \frac{\mu}{2\pi (1 - \nu)} \), \( \mu \) is the shear modulus, \( b \) is the signed magnitude of Burgers vector, \( \nu \) is Poisson’s ratio, \( \rho_a = \sqrt{x^2 + y^2 + a^2} \) and \( a \) is an arbitrary constant (core width).

For parallel slip plane with spacing of \( d \), shown in Fig. 2.2(a), dislocations dislocations \( i \) and \( j \) with magnitude of Burgers vector equals \( b_i \) and \( b_j \) respectively. The coordinate \( s_i \) is defined as the distance from the origin of the local slip plane to the dislocation \( i \). The change of interaction energy per unit length in parallel slip plane is

\[ \Delta E_{ij}^{\text{int}} (\Delta s_i, \Delta s_j) = -Ab_i b_j \left[ \frac{1}{2} \ln \left( \frac{\rho^2}{\rho_0^2} \right) - d^2 \frac{(2s_j - 2s_i + \Delta s_j - \Delta s_i) (\Delta s_j - \Delta s_i)}{\rho^2 \rho_0^2} \right] \] (2.4)

where \( \rho^2 = (s_j + \Delta s_j - s_i - \Delta s_i)^2 + d^2 + a^2 \) and \( \rho_0^2 = (s_j - s_i)^2 + d^2 + a^2 \). The interaction of intersecting slip plane with angle \( \theta \) can be derived in the similar way, as shown in Fig. 2.2(b). The coordinate \( s_i \) is the distance from the intersecting point to the dislocation \( i \). The change of interaction energy per unit length between dislocation \( i \) and \( j \) is given by
2.1. FORMULATION

\[ \Delta s_i, \Delta s_j \]

\[ R \]

\[ d \]

\[ \Delta \]

\[ s_i \]

\[ s_j \]

\[ \Delta s_i \]

\[ \Delta s_j \]

\[ R_0 \]

\[ \theta \]

\[ O \]

\[ \Delta E_{int}(s_i, s_j) = -Ab_i b_j \left\{ \frac{1}{2} \cos \theta \ln \frac{\rho^2}{\rho_0^2} + \sin^2 \theta \left[ \frac{(s_i + \Delta s_i)(s_j + \Delta s_j)}{\rho^2} - \frac{s_is_j}{\rho_0^2} \right] \right\} \]

\[ \Delta E_{int}(\Delta s_i, \Delta s_j) = -Ab_i b_j \left\{ \frac{1}{2} \cos \theta \ln \frac{\rho^2}{\rho_0^2} + \sin^2 \theta \left[ \frac{(s_i + \Delta s_i)(s_j + \Delta s_j)}{\rho^2} - \frac{s_is_j}{\rho_0^2} \right] \right\} \]

where \( \rho^2 = (s_i + \Delta s_i)^2 + (s_j + \Delta s_j)^2 - 2(s_i + \Delta s_i)(s_j + \Delta s_j) \cos \theta + a^2 \) and \( \rho_0^2 = s_i^2 + s_j^2 - 2s_is_j \cos \theta + a^2 \). When \( a = 0 \), (2.4) and (2.5) recovers to singular energy formula in [15].

The work done by the external stress is integration of the applied stress \( \tau_{app} \) along the slip plane. The incremental form of the external energy per unit length is

\[ \Delta E_i^{ext}(\delta s_i) = \int_0^{\delta s_i} \tau_{app}(\Delta s_i) d(\Delta s_i) \] (2.6)

In our model all other processes exclusive to glide - short range effects, thermally activated escape and dislocation climb - that change the energy of the system are modeled as discrete events which are defined by constitutive rules or by solving an auxiliary boundary value problem (e.g., diffusion). Our methodology largely follows
2.2 Implementation

We consider a two-dimensional plane strain crystalline solid with plastic deformation taking place by both glide and thermal activation of edge dislocations along a specified set of crystallographic directions. Attention is confined to quasi-static deformation and body forces are assumed to be absent. The basic assumptions are: (i) dislocation glide coupled with thermal activation is the mechanism of plastic deformation, (ii) elastic properties are assumed to be unaffected by dislocation motion within the crystal, (iii) outside the dislocation cores, the dislocation stress, strain and displacement fields are accurately described by linear elasticity.

2.2.1 Superposition framework

The solution of the mechanical boundary value problem is solved using the linear elastic superposition framework by Van der Giessen and Needleman [16]. A homogeneous body that contains \( n \) dislocations is decomposed into a infinite medium (\( \sim \) field) contains all the dislocations and a complementary problem without dislocations (\( \tilde{\sim} \) field), shown in Fig. 2.3. The \( \sim \) field is described by dislocation solution in infinite medium and image contribution on the boundary can be determine. The \( \tilde{\sim} \) field is solved by FEM where the boundary condition is the original boundary condition minus the image contribution in \( \sim \) field. The total strain energy \( \Delta E \) in and the Peach-Koehler force are obtained by the superposition of \( \sim \) field and \( \tilde{\sim} \) field.

The mechanical boundary value problem is loaded incrementally based on the strain rate and choice of time step \( dt \). After every loading step, (2.1) is solved to obtain equilibrium positions of dislocations, while simultaneously updating the \( \sim \)
2.2. IMPLEMENTATION

Figure 2.3: Decomposition of a linear elastic body containing a number of dislocation into a homogeneous infinite solid (~ field) and the complementary problem free of dislocation (~ field)

field, following which all short range effects are checked. This process repeated until no further events are activated. Since the glide time scale has been eliminated, the new algorithm can operate at wide range of strain rate.

2.2.2 Optimization

The optimization part receives a dislocation configuration and calculate the equilibrium positions for each unpinned dislocation as an output. A couple of regular DDD steps are performed which update the ~ field and ~ field simultaneously based on Van der Giessen and Needleman [16] superposition framework. Within the DDD step, dislocation velocity is obtained by the drag law and all short range effect is accommodated.

The strain energy is minimized using a damped dynamics method (FIRE) Bitzek et al. [92] modified to account for the constraints (2.1c). The energy minimization algorithm uses the following propagation rules (given initial values for tolerance force $F_{\text{min}}$, $\alpha = \alpha_{\text{start}}$, time step $\Delta t = 0.5 \Delta t_{\text{max}}$, dislocation position vector $\mathbf{x}$ and velocity vector $\mathbf{v} = 0$, ):

STEP1: For given $\mathbf{x}$, calculate $\mathbf{F} = -\nabla (\Delta E)$, $\mathbf{a} = \mathbf{F}/m_f$ and $\mathbf{v}$ using velocity verlet integrating scheme; check for convergence that $\max(|\mathbf{F}|) < F_{\text{min}}$.  

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STEP2: Move dislocation $\mathbf{x}$ based on $\mathbf{a}$ and $\mathbf{v}$. check for pinned to obstacle and annihilation.

STEP3: check for constraint violation of (2.1c); if yes, go to the last feasible $\mathbf{x}$ and $\mathbf{v}$ in STEP1; decrease time step $\Delta t \rightarrow 0.5\Delta t$; return to STEP1.

FIRE: calculate the power $P = \mathbf{F} \cdot \mathbf{v}$; scale velocity $\mathbf{v} \rightarrow (1 - \alpha) \mathbf{v} + \alpha \mathbf{F}|\mathbf{v}|$; if $P > 0$ and the number of steps since last time $P < 0$ is larger than $N_{\text{min}}$, increase the time step $\Delta t \rightarrow \min(\Delta t_{\text{inc}}, \Delta t_{\text{max}})$ and decrease $\alpha \rightarrow \alpha f_{\alpha}$; if $P < 0$, decrease time step $\Delta t \rightarrow \Delta t_{\text{dec}}$, freeze the system $\mathbf{v} \rightarrow 0$ and set back $\alpha \rightarrow \alpha_{\text{start}}$; return to STEP1.

We would emphasize that $\Delta t$ and $\mathbf{v}$ here are minimization parameters and don’t have any physical meaning. So the dislocation motion in energy minimization does not reflect the actual dislocation dynamics. Other FIRE parameters are: $\Delta t_{\text{max}} = 0.2 \sim 2, m_f = 10^{-6}, \alpha_{\text{start}} = 0.2, f_{\text{inc}} = 1.05, f_{\text{dec}} = 0.5, N_{\text{min}} = 5$ and $f_{\alpha} = 0.9$. The choice of $\Delta t_{\text{max}}$ will affect the total number of iteration.

It is noted that the time in FIRE is totally fictitious and has no physical meaning. So the choice of FIRE time step is based on a couple of optimization test case of dislocation ensemble such that the average iteration is around $100 \sim 200$ steps. Also, a maximum velocity is used to prevent over shot.

2.2.3 Short range effects

After each minimization, all short range effects are handled using constitutive rules, first developed by Kubin [31] and implemented by Van der Giessen and Needleman [16]. The short range effects here refers to nucleation, annihilation, moving to the free surface and escaping from obstacle.

Dislocations are nucleated at point sources with a strength $\tau_s$ on the slip plane. A dislocation dipole spaced equally about the source is generated when the stress at the source location is greater than the source strength $\tau_s$. The initial equilibrium
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separation \( L_{\text{nuc}} \) is given by
\[
L_{\text{nuc}} = \frac{\mu b}{\pi (1 - \nu) \tau_s} \frac{1}{\tau_s},
\]
where \( \mu \) is the shear modulus, \( b \) is the signed magnitude of Burgers vector and \( \nu \) is Poisson’s ratio. This ensures that the dipole is in equilibrium when the stress is equal to \( \tau_s \). The equilibrium separation of a source \( L_{\text{nuc}} \) also defines a dislocation-free zone. In our implementation, we test if a virtual dipole located at \( L_{\text{nuc}}/2 \) on either side of the source will move towards each other. Nucleation of a new dipole is performed only if the two virtual dislocations tend to move apart.

Annihilation occurs when the distance between two dislocations with opposite sign is less than a critical value. Here we used \( 4b \). Escaping from obstacle event happens when the stress acting on the pinned dislocation is greater than the obstacle strength. The pinned dislocation will be released from that obstacle. When dislocation is closing to the free surface less than \( 4b \). It will be removed from the body and created a step on the surface. As in standard 2d DDD we treat obstacles as points on the slip plane with a strength \( \tau_{\text{obs}} \) which impedes dislocation glide. A dislocation pinned by an obstacle will be released when the shear stress on the obstacle is greater than its strength and this is considered athermal escape.

2.2.4 Algorithm procedure

The mechanical boundary value problem is loaded incrementally based on the strain rate and choice of time step \( dt \). After every loading step, (2.1) is solved to obtain equilibrium positions of dislocations, following which all short range effects are checked. In order to accommodate thermal activation, the loading time step is subdivided into several thermal time steps (\( O(10) \)) over which thermal activation is evaluated. In the event of thermal activation, (2.1) is solved again to re-evaluate equilibrium positions. This process repeated until no further events are activated. In general, for the range of strain rates and temperatures considered in this study we found that the modified
2.3. ALGORITHM VALIDATION

FIRE solver is capable of solving (2.1) in less than 200 iterations. Since the glide time scale has been eliminated, simulation of rate-controlled thermal processes over the entire range of parameters studied here can be achieved with the same amount of computational cost by scaling the time step inversely with strain rate. Therefore, the new algorithm is able operate at a wide range of strain rates without any appreciable change in computational time.

2.3 Algorithm validation

In the this section, we will compare the new algorithm with the analytical solution as well as DDD result.

2.3.1 Dislocation pileup

Here we consider a source with strength \( \tau_s \) surrounded by two equally-spaced obstacles with strength \( \tau_{\text{obs}} \), shown in Fig. 2.4. A uniform shear stress \( \tau_{\text{app}} \) that increases linearly with time is applied. When the shear stress on the source is greater than \( \tau_s \), a dislocation dipole is nucleated. The two dislocations move apart under applied shear stress until they get pinned by the obstacles. With increasing applied stress, more dislocations are generated and a pile-up is formed. Eventually, when the shear stress on the pinned dislocation is greater than \( \tau_{\text{obs}} \), the dislocation escapes from the obstacle and macroscopic flow begins. Here we define the yield stress \( \tau_Y \) as the applied shear stress required for a dislocation to escape from the obstacle. The relationship between yield stress as a function of obstacle spacing and strength is given by [93].

\[
\tau_Y = \sqrt{\frac{4\mu b}{\pi (1-\nu)} \frac{\tau_{\text{obs}}}{L_{\text{obs}}} + \tau_s^2} \quad (2.7)
\]
2.3. ALGORITHM VALIDATION

Figure 2.4: Schematic of 1d pile-up, showing source and obstacles in a linear applied stress gradient

Figure 2.5: Predicted yield stress by (2.7) vs. actual yield stress from the new algorithm for 1d pile-up. The error is less than 5%.

Figure 2.5 shows the comparison of the yield stress obtained simulations and those predicted by (2.7) for a three different values of $L_{\text{obs}}$ and a wide range of $\tau_s$ and $\tau_{\text{obs}}$. In this figure, the elastic modulus $E = 70$ GPa, Poison’s ratio $\nu = 0.33$ and the magnitude of Burgers vector $b = 0.25$ nm. The source strength $\tau_s = 50$ MPa. Three different $L_{\text{obs}}$ are used, 0.2 $\mu$m, 0.4 $\mu$m and 0.6 $\mu$m. Obstacle strength $\tau_{\text{obs}}$ is chosen from 200 MPa to 2 GPa. The simulations results are within 5% of (2.7), demonstrating that the new algorithm is capable of modeling all the key material dependencies of the flow stress accurately.
2.3. ALGORITHM VALIDATION

2.3.2 Uniaxial tension in single crystal

Further validation with multiple sources and obstacles on multiple slip planes is performed. A rectangular sample of $6 \, \mu m \times 1 \, \mu m$ is studied with multiple sources and obstacles on multiple slip systems, shown in Fig. 2.6. The crystallography is represented by three slip systems with angles equal to $\varphi_1 = 30^\circ$, $\varphi_2 = 150^\circ$ and $\varphi_3 = 90^\circ$. The elastic modulus is $E = 70$ GPa, Poisson’s ratio is $\nu = 0.33$ and the magnitude of Burgers vector $b = 0.25$ nm. Sources are randomly distributed with a density of $25 \, \mu m^{-2}$. Each source is randomly assigned a nucleation strength from a Gaussian distribution with a mean of $\tau_s = 50$ MPa and a standard deviation $\Sigma_s = 0.2\tau_s$. Obstacles are generated on each slip plane from a uniform distribution with a mean of $L_{obs}$, a minimum of $0.5L_{obs}$ and a maximum of $1.5L_{obs}$ [93]. For each $L_{obs}$ and $\tau_{obs}$, simulations of three different statistical distributions of sources and obstacles were performed.

The yield stress for these types of obstacle controlled configurations has been predicted analytically by Chakravarthy and Curtin [93] as,

$$
\sigma_Y = \frac{1}{M} \sqrt{\frac{4\mu b}{\pi (1 - \nu)}} \frac{\tau_{obs}}{1.5L_{obs}} + \tau_s^2
$$

(2.8)
where $M$ is the Schmidt factor for the dominant slip systems, $\tau_s = \bar{\tau}_s - 2\Sigma_s$. We chose $L_{\text{obs}} = 0.2, 0.4, 0.6 \, \mu m$ and $\sigma_Y = 300 \, \text{MPa}$. Obstacle strength is calculated from (2.8) for each $L_{\text{obs}}$. We first run a DDD simulation using the input above. The DDD time step is chosen as $5 \times 10^{-11} \, \text{s}$ and strain rate $\dot{\varepsilon} = 1000 \, \text{s}^{-1}$. The dislocation is moved by drag law (1.2) where $B = 4 \, \text{Pa} \cdot \text{s}$ [16] and Peach-Koehler force along the slip plane $F$ is calculated by (2.2). Then we ran the same strain rate using $dt = 10^{-6} \, \text{s}$.

The stress-strain response of the sample is shown in Fig. 2.7(a) for both pure 2d DDD simulations and the new algorithm simulations performed with $L_{\text{obs}} = 0.2 \, \mu m$ and $\tau_{\text{obs}}$ chosen according to (2.8) such that $\sigma_Y = 300 \, \text{MPa}$. The overall response for both simulations is extremely similar, with the new algorithm exhibiting slightly higher yield stress. Figure 2.7(a) also shows the evolution of dislocation density with applied strain, which shows that the new algorithm simulations have nearly identical dislocation density to DDD simulations. Figure 2.7(b) shows comparison of snapshots of dislocation patterns and Fig. 2.7(c) showing a close up view corresponding the marked black box in Fig. 2.7(b). The dislocation patterns are nearly identical, demonstrating that the new algorithm essentially captures all features of DDD without actually having to follow the dislocation path as the system evolves. The new algorithm simulations are insensitive to the choice of $dt$ and the chosen value was used only to obtain a sufficiently representative stress vs strain curve. We have performed simulations with $dt$ varying from $10^{-8}$ to $10^{-3} \, \text{s}$ and found no discernible difference in dislocation configurations.

Later we run $\dot{\varepsilon} = 0.01, 0.1, 1, 10, 100 \, \text{s}^{-1}$ by scaling $dt$ proportionally with respect to the $1000 \, \text{s}^{-1}$ case. Figure 2.8(a) shows the number of force evaluations as a function of strain at $L_{\text{obs}} = 0.2 \, \mu m$ when $\dot{\varepsilon} = 0.01 \, \text{s}^{-1}$. The average function call per strain is about 400 and half of them spend on obstacle escape. Then we summarize all the cases and plot number of force evaluations as a function of strain rate in Fig. 2.8(b).
2.4. **Summary**

The excellent agreement between DDD and the new algorithm illustrated in Fig. 2.5 and Fig. 2.7, validates the energy minimization strategy. This is the first main result of presented work. The framework to finding equilibrium positions of dislocations is similar to equations and methodology proposed in [15]. However, that model and other similar models have not implemented the short range interactions. They have only been applied to problems in which the desired result is the equilibrium configurations of dislocations, for a given initial configuration of dislocations. Also in
Figure 2.8: Number of force evaluation as a function of strain rate under different $L_{obs}$.
[15] several equilibria exist for a given initial configuration. While we have not avoided the problem, our analysis always finds the nearest local minimum for dislocations for a given increment. Our approach closely follows the dislocation dynamics approach without actually tracking the position of dislocations as they move. This allows for an arbitrary choice of time increments. Also, because the glide time scale has been eliminated, the new algorithm has a large flexibility in changing the time scale, which pave the way to incorporate thermal activation or other thermal process.
CHAPTER 3

THERMALLY ASSISTED DISCRETE DISLOCATION

For a system in which the total strain energy is minimized, dislocations are either in equilibrium or pinned against obstacles. Thermal activation can now be incorporated at the appropriate time scales. We adopt a general energy formula to characterize the thermal activation over obstacle and establish a new framework to fill the gap between dislocation glide and thermal activation. We call this new model thermally assisted discrete dislocation (TADD). This chapter will describe the formulation and implementation of TADD as well as its validation and application.

3.1 Formulation

This section introduces the characterization of thermally assisted escape from obstacle field and the thermal activation strategy.

3.1.1 Thermal activation over obstacle

In general the process of a dislocation line bypassing an obstacle field (solute, precipitates, forest dislocations) can be characterized by a dislocation-obstacle interaction
energy and a coherent sampling length [49], which is the effective distance between obstacles on the slip plane intersecting the dislocation line as it moves, shown in Fig. 3.1. The dislocation-obstacle interaction energy establishes the relationship between the obstacle resistance to dislocation motion under an applied stress. It has been extensively studied and accurate models have been formulated for a variety of obstacles: solid solution strengthening [43, 44, 46], precipitation strengthening [29, 45, 94], dynamic strain aging [95, 96] and superposition of different types of obstacles [26, 54, 97]. Consider a dislocation passing through an obstacle group as shown schematically in Fig. 3.1. Each individual obstacle has different energy barrier $\Delta G$. However, the thermal activation of the dislocation front can still be described by a mean activation energy $\Delta G^*$ [50], and the average frequency of escape $f$ is given by

$$f = f_{\text{eff}} \exp \left\{ -\frac{\Delta G^* (\tau, \tau_{\text{obs}}, \ldots)}{k T} \right\}$$

(3.1)

where $\tau$ is the stress on the obstacle, $\tau_{\text{obs}}$ is the threshold shear resistance, $k$ is Boltzmann constant, $T$ is the temperature and $f_{\text{eff}}$ is on the order of the Debye frequency. $\Delta G^*$ depends on the nature and size of the obstacles, their distribution on the slip plane and the nature of dislocation interaction, which can be chosen from a variety of existing models [43, 44, 45, 46, 94, 98] or from atomistic simulations. The probability density per unit time for a dislocation to escape at time $t$ is defined by the instantaneous rate of attempt [95]

$$p (\tau, t) = f (\tau (t), t) e^{-\gamma (t)}$$

(3.2)

with

$$\gamma (t) = \int_0^t f (\tau (t'), t') \, dt'$$

(3.3)
3.1. FORMULATION

Figure 3.1: Schematic of thermal activation of a 3d dislocation line over an obstacle spectrum, with the dark black line representing a dislocation getting pinned and bowing out due to obstacles and the red showing thermal stochastic activation of a few segments. The free energy barrier $\Delta G^*$ in 2d represents the interaction between a dislocation segment and obstacles averaged over the coherent length.

In the context of two dimensions, where the entire dislocation line and the obstacles encountered by it are represented by points, modeling stochastic thermal activation over individual obstacles is not trivial. In our view the obstacle strength $\tau_{\text{obs}}$ in 2d represents the stress equivalent resistance of distributed obstacles along the dislocation line (Fig. 3.1). In addition the average in-plane obstacle spacing $L_{\text{obs}}$ is a function of coherent sampling length and the average actual spacing of obstacles. We treat $\tau_{\text{obs}}$, $L_{\text{obs}}$ and $\Delta G^*$ as adjustable nano-scale input parameters to our analysis. We now define thermal activation in 2d as the average time required for a straight dislocation to bypass an obstacle. Then the waiting time is average of the entire
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The deterministic 2d thermal escape model can thus be viewed as a statistical average of the three-dimensional stochastic process. Equation (3.4) is the general definition of waiting time.

### 3.1.2 Evaluation of average waiting time

Without losing the generality of $\triangle G^*$, we value (3.4) in two categories: $\Delta G^*$ is not explicitly dependent on time and $\Delta G^*$ is a function of time.

#### The free energy barrier $\Delta G^*$ is independent of time

Let $\Delta G^* = \Delta G^* (\tau, \tau_{obs})$ and by (3.3), $\gamma$ can be simplified to

$$\gamma (t) = \int_0^\infty f (\tau) \, d\tau$$

then wait time can be exactly solved

$$t_w = \int_0^\infty e^{-\gamma(t)} \, dt = \frac{1}{f(\tau)}$$

Then the average waiting time $t_w$ of a dislocation sitting in front of the obstacle is the inverse of the $f$
3.1. FORMULATION

\[ t_w = t_{\text{min}} \exp \left\{ \frac{\Delta G^* (\tau, \tau_{\text{obs}})}{kT} \right\} \]  \hspace{1cm} (3.7)

where \( t_{\text{min}} = 1/f_G \) is the minimum waiting time. One step further, Kocks et al. [25] fit different mechanisms broadly to a general empirical expression

\[ \Delta G^* = \Delta G_0^* \left[ 1 - \left( \frac{\tau}{\tau_{\text{obs}}} \right)^p \right]^q \]  \hspace{1cm} (3.8)

where \( \Delta G_0^* \) is free energy barrier at 0 K and the exponents \( p \) and \( q \) are generally in the range of

\[ 0.5 \leq p \leq 1.0 \]
\[ 1.0 \leq q \leq 2.0 \]  \hspace{1cm} (3.9)

Therefore, Equation (3.7) can be further simplified as

\[ t_w = t_{\text{min}} \exp \left\{ \frac{\Delta G_0^*}{kT} \left[ 1 - \left( \frac{\tau}{\tau_{\text{obs}}} \right)^p \right]^q \right\} \]  \hspace{1cm} (3.10)

The free energy barrier \( \Delta G^* \) is a function of time

It is difficult to get a close form expression for \( t_w \). Here we use approximation of \( t_w \) proposed by [97]. From (3.4a) we can write

\[ t_w = \int_0^{t_0} t \cdot f (\tau (t), t) e^{-\gamma(t)} dt + \int_{t_0}^{\infty} t \cdot f (\tau (t), t) e^{-\gamma(t)} dt \]  \hspace{1cm} (3.11)

Since we now choose \( t_0 \) such that \( \gamma(t_0) = 1 \). We assume that \( f(t) \) to be increasing monotonically with \( t \), it follows that \( \gamma(t) \) increases faster than linear function \( t \). Therefore the second term in (3.11) is smaller than first term but they may be in the same order. For the first integral, it can be rewritten as

\[ \int_0^{t_0} t \cdot f (\tau (t), t) e^{-\gamma(t)} dt = C \int_0^{t_0} t \cdot f (\tau (t), t) dt \]  \hspace{1cm} (3.12)
with $1/e < C < 1$. Integrating by part gives

$$\int_0^{t_0} t \cdot f (\tau (t), t) \, dt = t_0 \gamma (t_0) - \int_0^{t_0} \gamma (t) \, dt$$

(3.13)

since $\gamma (t)$ is stronger than linear in $t$ the integral on the right-hand side of (3.13) is equal to $p \gamma (t_0) t_0$ with $p < 1/2$. Substituting (3.12) and (3.13) into (3.11), we have

$$t_w = C (1 - p) \gamma (t_0) t_0 + O (t_0)$$

(3.14)

since we have chosen $t_0$ such that $\gamma (t_0) = 1$ we find from (3.14) that $t_0 \approx t_w$ and hence

$$\gamma (t_w) = \int_0^{t_w} f (t) \, dt \approx 1$$

(3.15)

The physical interpretation of (3.15) is that after $t_w$ most of the thermal activation have taken place. Also the upper and lower bound for this approximation is $[0.2 e, 1]$.

### 3.1.3 Thermal activation strategy

Practically, thermal activation is treated as a discrete event for non-equilibrium dislocations that are pinned at obstacles. The waiting time can be computed analytically for various types of obstacles and physical mechanisms such as solid-solution strengthening or precipitation strengthening. Each dislocation is associated with a residence time $t$ that is accumulated when a dislocation is pinned against obstacles and reset to zero when it moves again. A dislocation can thermally pass an obstacle when the waiting time of each pinned dislocation at its current loading and temperature is greater than its residence time. The residence time for a dislocation depends on the
3.2. IMPLEMENTATION

3.2 Implementation

The mechanical boundary value problem is loaded incrementally based on the strain rate and choice of time step $dt$. After every loading step, (2.1) is solved to obtain equilibrium positions of dislocations, following which all short range effects are checked. In order to accommodate thermal activation, TADD is divided into two layers of loops: inner loop accounts for an event that has much less time scale comparing with $dt$ such as short range effect. When no event happens, we jump to the outer loop which accounts for an event that has the same order or one order less than $dt$ ($dt/20 \sim dt$). Whenever a thermal event occurs, we first enter inner loop and accounting all of them and then check the next thermal events. In the event of either loop, (2.1) is solved again to re-evaluate equilibrium positions. This process repeated until no further events are activated before moving to the next loading step.

3.3 Numerical results

In order to qualify the TADD algorithm, we test it on pileup and uniaxial tension

3.3.1 Finite temperature results in pileup

TADD simulations were performed to examine thermal activation over an obstacle. We start by examining the 1d pile-up described in Section 2.3.1. For a constant applied shear strain rate $\dot{\gamma}$ along the slip plane, the applied stress $\tau_{\text{app}}$ varies linearly with residence time $t$, written as $\tau_{\text{app}} = \mu \dot{\gamma} (t + t_0)$ where $t_0 = \tau_s / \mu \dot{\gamma}$ is the time
3.3. NUMERICAL RESULTS

Figure 3.2: The procedure of TADD. The blue par the is inner loop that accounting for all the athermal event. Outer loop in orange accounts for the thermal event takes place comparable with $dt$

required to nucleate the dislocation dipole for a source with strength $\tau_s$. Then the resident time $t$ is

$$t = \frac{\tau_{\text{app}} - \tau_s}{\mu \dot{\gamma}}$$  \hspace{1cm} (3.17)

The relationship between the applied stress $\tau_{\text{app}}$ and stress on the leading dislocation $\tau$ in the pile-up will follow that of (2.7)

$$\tau_{\text{app}} = \sqrt{\frac{4\mu b}{\pi (1 - \nu) L_{\text{obs}}} \tau + \tau_s^2}$$  \hspace{1cm} (3.18)
By substituting (3.18) into (3.17), we have the relationship between resident time \( t \) and stress on the obstacle \( \tau \)

\[
    t = \frac{1}{\mu \dot{\gamma}} \left[ \sqrt{\frac{4\mu b}{\pi (1 - \nu) L_{obs}}} \frac{\tau}{L_{obs}^2 - \tau_s^2} \right]
\]

(3.19)

Also by dividing both sides of (3.18) by (2.7), the relationship between applied stress \( \tau_{app} \) and stress on the obstacle \( \tau \) is as follows

\[
    \frac{\tau}{\tau_{obs}} = \left( \frac{\tau_{app}}{\tau_Y} \right)^2 - \left( \frac{\tau_s}{\tau_Y} \right)^2 \over 1 - \left( \frac{\tau_s}{\tau_Y} \right)
\]

(3.20)

Our implementation of thermal activation is general for any obstacle type, and the activation energy barrier \( \Delta G^* \) in (3.7) can take any functional form or can be obtained from atomistic simulations of dislocation obstacle interactions. To illustrate thermal activation behavior in a pileup, we choose \( \Delta G^* \) corresponding to solid solution strengthening (SSS) model [98], treating \( \tau_{obs} \) and \( L_{obs} \) as parametric inputs to the model. According to the SSS model

\[
    \Delta G^* = \Delta G_0^* \left( 1 - \frac{\tau}{\tau_{obs}} \right)^{\frac{3}{2}}
\]

(3.21)

where

\[
    \Delta G_0^* = 5.55 \left( \frac{\mu b^3}{w} \right) \left( \frac{w}{b} \right)^{\frac{3}{2}} \left( \frac{\tau_{obs}}{\mu} \right)^{\frac{1}{2}}
\]

(3.22)

and \( w = 1.7b \) is the range of the solute interaction. By substituting (3.21) into (3.7), the average waiting time for any dislocation pinned at an obstacle is determined to be

\[
    t_w = t_{\text{min}} \exp \left[ \frac{\Delta G_0^*}{kT} \left( \frac{\tau_Y^2 - \tau_{app}^2}{\tau_Y^2 - \tau_s^2} \right)^{\frac{3}{2}} \right]
\]

(3.23)
Then the unknown yielding stress $\tau_{\text{app}}$ at given strain rate $\dot{\gamma}$ and temperature $T$ can be solved using (3.16), (3.19) and (3.23).

Numerical simulations were performed for a range of $L_{\text{obs}} = 0.2$, 0.4 and 0.6 $\mu$m, $\tau_{\text{obs}}$ from 400 MPa to 1.8 GPa and $\tau_s = 50$ MPa. Also for six different strains rates $\dot{\gamma}$ ($0.01$ s$^{-1}$, $0.1$ s$^{-1}$, $1$ s$^{-1}$, $10$ s$^{-1}$, $100$ s$^{-1}$, $1000$ s$^{-1}$) and three different temperatures (300 K, 600 K, 900 K) are tested. The elastic modulus $E = 70$ GPa, Poison’s ratio $\nu = 0.33$ and the magnitude of Burgers vector $b = 0.25$ nm. Figure 3.3(a) shows plot of the dislocation residence time plotted against the non-dimensional applied stress $(\tau_{\text{app}}/\tau_Y)$. The solid black lines represent plot of residence time, given by (3.17) of a dislocation at an obstacle at different strain rates and the colored lines are a plot of (3.23). The dashed lines from (3.19) represent the numerical results of stress on obstacle $\tau$ in terms of dislocation residence.

The intersection between the curves of (3.17) and (3.23) represents the stress/time at which a dislocation will be thermally activated over the obstacle. For the same temperature, the intersecting point of the lower strain rate curve gives lower yielding stress. This implies a positive rate sensitivity. For the same strain rate, higher temperatures will predict lower yielding stress, which indicates a thermal effect. Fig. 3.3(a) provides guidance for choosing $dt$. For a strain rate of $1000$ s$^{-1}$, all the thermal activation occurs at times greater than $10^{-6}$ s, making $dt = 10^{-8}$ s sufficiently accurate to capture all thermal effects.

The simulation data is not smooth, due to the discrete nature of the dislocations. The first dislocation is nucleated and the residence time grows smoothly with applied stress, however there is a sudden jump in the stress when the second dislocation in nucleated with subsequent jumps for every dislocation that joins the pileup. This is clearly seen in Fig. 3.3(b), where $L_{\text{obs}} = 0.2$ $\mu$m and $\tau_{\text{obs}} = 400$ MPa at 600 K. Since the stress on the pinned dislocations in a pile-up grows approximately as $n\tau_{\text{app}}$, the magnitude of these discontinuities decreases with increasing number of dislocations in
3.3. NUMERICAL RESULTS

Figure 3.3: Thermal activation of dislocations in a pileup showing (a) Dislocation residence time plotted vs normalized applied stress for $L_{\text{obs}} = 0.2 \mu$m and $\tau_{\text{obs}} = 800$ MPa. Black solid lines show the timer predicted by (3.17) under different strain rate and dashed line is the timer in a TADD simulation. Colored lines are the waiting time given by (3.23) at 300 K, 600K and 900 K. Intersection of solid lines gives the analytical prediction of thermally activated escape and dots are the actual activation points in the simulation, illustrating the thermal activation strategy of TADD; (b) The discrete nature of dislocations and its effect on thermal activation at $L_{\text{obs}} = 0.2 \mu$m and $\tau_{\text{obs}} = 400$ MPa (c) Predicted vs actual normalized shear yield stress for $\tau_{\text{obs}} = 400 \sim 1800$ MPa, where the shaded region represents a 5% error.

the pileup (or increasing $\tau_{\text{obs}}$). Figure 3.3(c) shows a plot of the flow stress by TADD normalized by the zero temperature flow stress versus values predicted by the pile-up model and empirical law normalized by (2.7). The gray shaded region represents a 5% error. It can be seen that actual yield stress is within 5% of the predicted value for the entire parametric range. It should also be noted that when the number of dislocations in the pileup is small the predicted values overestimate the actual yield stress. Figure 3.3 shows that our model is capable of capturing all the mechanistic aspects of thermally activated escape from obstacles and is the second main result of this paper.
3.3. NUMERICAL RESULTS

3.3.2 Uniaxial tension in single crystal

TADD simulations were performed with thermal activation enabled in uniaxial tension. The geometry of the sample, boundary conditions and elastic properties are identical to those described in Section 2.3.2. The obstacle strength is calculated by (2.8) with \( \sigma_Y = 300 \) MPa and thermal activation is performed according to the energy barrier in (3.21). The results are averaged over three different statistical configurations of sources and obstacles.

Similar to Section 3.3.1, the predicted yield stress at a given temperature and strain rate is obtained by solving (3.7),

\[
\sigma_{\text{app}} = \frac{(1 - \nu) E \dot{\varepsilon}}{(1 + \nu) (1 - 2\nu)} t + \frac{\tau_s}{M}
\]

and

\[
t_w = t_{\text{min}} \exp \left[ \frac{\Delta G^*_0}{kT} \left( \frac{\sigma_Y^2 - \sigma_{\text{app}}^2}{\sigma_Y^2 - \sigma_s^2} \right)^{\frac{3}{2}} \right]
\]

which is derived similarly with (3.23). Figure 3.4(a) shows the yield stress obtained in TADD simulations versus the predicted values. The error between simulated results and predicted is less than 5% shown by the shaded region in Fig. 3.4(a). Positive rate sensitivity is observed with the flow stress increasing with strain rate and vice versa. At a given temperature, lower strain rates allow more time for dislocations to be pinned at the obstacle at a given stress, thereby enabling more frequent thermal escape and thus plastic flow at a lower stress. As the temperature goes up, the effect of strain rate on the flow stress increases. Since higher temperatures require less average waiting time for the same free energy barrier, more dislocations will be thermally released from obstacles. The thermal effects are even more obvious than rate effects, depicted in Fig. 3.4(c) in which the axial definition is the same as Fig. 3.4(b). The correlation between rate effects and thermal effects have been illustrated
3.3. NUMERICAL RESULTS

Figure 3.4: Numerical results for a TADD simulation with \( L_{\text{obs}} = 0.2 \mu m \) and zero temperature yield stress \( \sigma_Y = 300 \) MPa (a) Predicted vs actual normalized stress under different loading rates and temperatures with shaded region representing 5% error (b) Normalized stress vs strain at 300 K and 900 K at different strain rates (c) Normalized stress vs strain at \( 10^{-2} \) s\(^{-1} \) and \( 10^{3} \) s\(^{-1} \) at different temperatures.

by Fig. 3.3(a). Higher temperatures will enhance the rate effects and lower strain rates will exhibit more significant thermal effects.

Not all pinned dislocations are capable of thermally activated from obstacles. In order to investigate this, we plot number of athermal escaped dislocation and thermally activated dislocation normalized by the number of pinned dislocation, shown in Fig. 3.5(a). Only less than 3% pinned dislocations are escaped and only less than 20% escaped dislocation are through thermal activation. Also both the athermal escape and thermal activation are quit stochastic for a certain range of strain. To get a clear portion of it. The ratio is averaged over 0.002 to 0.04 strain shown in Fig. 3.5(b) and the averaged ratio is summarized by strain rate and temperature in Fig. 3.6. We see that the portion of athermal escaped dislocation dramatically decrease under finite temperature whereas the portion of thermally activated dislocation has opposite
3.3. NUMERICAL RESULTS

Figure 3.5: (a) Ratio of athermal escaped dislocation no. over pinned dislocation no. (red) and thermally activated dislocation no. over pinned dislocation no. (green) as a function of strain at $L_{obs} = 0.2 \, \mu m$, $\dot{\varepsilon} = 1000 \, s^{-1}$ and $T = 300 \, K$; (b) Averaged ratio from strain $0.002 \sim 0.04$ of (a)

trend but not sensitive to the temperature. Also, at high strain rate, athermal escape is tend to increase while thermal activation is decrease. All these observation agree with the thermal effect and rate effect shown in Fig. 3.4.

To measure the performance of TADD, we count for the no. of force evaluation in Fig. 3.7. The total force is summarized in Fig. 3.6, showing the computational cost remains the same amount over 6 order of magnitude in strain rate and three different obstacle spacing.

Assuming a classical power law relationship between the flow stress, strain rate and temperature [99], the strain rate sensitivity parameter $m$ [95, 100] is given by

$$m = \frac{d (\ln \sigma_Y)}{d (\ln \dot{\varepsilon})} \quad (3.26)$$
3.3. NUMERICAL RESULTS

Figure 3.6: Averaged ratio escaped dislocation (red) and thermally activated dislocation (green) at $L_{\text{obs}} = 0.2 \, \mu\text{m}$ under four different temperatures

Figure 3.7: No. of force evaluation as a function of strain at $L_{\text{obs}} = 0.2 \, \mu\text{m}$ at $\dot{\varepsilon} = 0.01, 1000 \, \text{s}^{-1}$ and $T = 0, 300, 900 \, \text{K}$
3.3. NUMERICAL RESULTS

Figure 3.8: Number of force evaluation as a function of strain rate under different temperature for $L_{\text{obs}}$ (a) 0.2 µm, (b) 0.4 µm and (c) 0.6 µm

where $\sigma_Y$ is the flow stress for a given temperature and strain rate. Fig. 3.9 shows a plot of $\sigma_Y$ versus $\ln \dot{\varepsilon}$ at different temperatures, with each point on the plot representing $\sigma_Y$ for a single statistical distribution. $\sigma_Y$ is obtained from a curve fit of the elastic-plastic transient regime. Figure 3.9 clearly shows that there are no rate effects at 0 K and the flow stress increases with strain rate at all other temperatures. The material with the chosen $\Delta G^*$ using (3.21) clearly displays a positive rate sensitivity. The inset in Fig. 3.9 shows the variation of $m$ with temperature, showing that strain rate sensitivity exponent increases with temperature. Capturing positive rate sensitivity for dislocation ensembles in tension, is the third main result of this paper.

Figure 3.10 summarizes our data over all the obstacle spacing, strain rates and temperatures considered in this study. The predicted results are within 5% of the analytically predicted data for the flow stress. TADD demonstrates a good agreement with analytical solution. For finite temperature simulations, $dt$ was chosen according using the strategy described earlier, which approximately amounts to scaling the increment with inverse of the strain rate. The entire set of our simulations requires
3.3. NUMERICAL RESULTS

Figure 3.9: Flow stress $\sigma_Y$ plotted vs. strain rate for different temperatures at $L_{obs} = 0.2 \mu$m, clearly showing positive rate sensitivity. The inset plot shows the variation of strain rate sensitivity exponent with temperature.

approximately the same computational effort and is relatively independent of temperature and strain rate, allowing simulation of rates not accessible to DDD simulations before.

3.3.3 Bending of single crystal for multi-slip

Bending cases are also examined. The simulation parameter takes from Section 3.3.2, except the applied load has a gradient accounting for pure bending, shown in Fig. 3.11. The obstacle model is (3.21) and (3.22). The stress on the top surface is monitored, which is normalized by the initial yield stress at zero temperature.

Figure 3.12(a) shows the rate effects under different temperature and obstacle spacing. The horizontal axis is the normalized surface stress and vertical axis is the surface strain. At 300 K, initial yield stress in $L_{obs} = 0.2 \mu$m decrease about 10 % when the strain rate changes over 6 order of magnitude. The rate effect becomes more significant at high temperature. At 900 K, the initial yield stress drops
3.3. NUMERICAL RESULTS

Figure 3.10: Predicted vs actual normalized stress, obstacle spacing $L_{\text{obs}} = 0.2 \mu m \sim 0.6 \mu m$, strain rate $\dot{\varepsilon} = 0.01 \text{ s}^{-1} \sim 1000 \text{ s}^{-1}$ and temperature $T = 0 \text{ K} \sim 900 \text{ K}$, with shaded region representing a 5% error.

Figure 3.11: Geometry and boundary conditions of the TADD algorithm problem with three active slip systems, loaded in pure bending.
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Figure 3.12: Normalized surface stress vs surface strain under different loading rate for bending cases of $L_{obs} = 0.2 \mu m$ (a) strain rate from 0.01 to 1000 s$^{-1}$ at 300 K and 900 K, (b) temperature from 0 to 900 K at strain rate 0.01 and 1000 s$^{-1}$

about 20 % in 0.2 $\mu m$. Figure 3.12(b) shows the thermal effects under the different temperature. In $\dot{\varepsilon} = 0.01$ s$^{-1}$, the initial yield stress in 0.2 $\mu m$ decreases about 36%. Both rate effects and thermal effects are observed under a wide range of strain rate and temperature.
3.3.4 Crack growth

The fracture problem has been studied by DDD, without combining the thermal activation. Next we will examine the crack growth problem under finite temperature. A common approach to modeling crack growth in both DDD and continuum plasticity is through the use of a cohesive zone model as a continuum model of the complex nonlinear separation. The cohesive zone have two primary properties: the cohesive strength $\sigma_{coh}$, ranging from 2 to 20 GPa, and the fracture energy $\Gamma_0$, typically a few Jm$^{-2}$. Continuum plasticity models predict no crack growth in the regime $\sigma_{coh}/\sigma_Y > 3-5$ [101] which is typically exceeded in most realistic materials and has thus driven the application of strain gradient plasticity or DDD model. Two characteristic lengths associated with the cohesive zone are the critical opening $\delta_n \sim \Gamma_0/\sigma_{coh}$, typically 0.1 nm and thus comparable to the dislocation Burgers vector, and the critical cohesive length $\delta_{coh} \sim \mu \Gamma_0/\sigma_{coh}^2$, typically 1 nm.

The elastic modulus $E = 70$ GPa, Poisson’s ratio $\nu = 0.33$ and the magnitude of Burgers vector $b = 0.25$ nm. A upper half model is chosen with a per-existing crack and loaded by mode-I stress intensity $K$, shown in Fig. 3.13. The size of the upper half model is 1000×500 $\mu$m which contains a process window with size 20×20$\mu$m. Within the process window, three slip systems with angles equal to 60°, 120° and 0° are used and slip plane spacing with 100$b$ is generated. Sources which has a mean of $\tau_s = 50$ MPa and a standard deviation $\Sigma_s = 0.2\tau_s$ are randomly distributed with a density of 66 $\mu$m$^{-2}$. Obstacles are generated on each slip plane from a uniform distribution with a mean of $L_{obs} = 80$ nm, a minimum of $0.5L_{obs}$ and a maximum of $1.5L_{obs}$. The obstacle is assigned following (2.8), where yielding stress $\tau_Y = 500$ MPa. In front of the crack tip, a cohesive zone is introduced to account for the crack opening and propagation. The mode-I crack boundary condition involves imposing a
remote displacement field which is

\[
\begin{align*}
    u_x &= \frac{K}{\mu} \sqrt{\frac{r}{2\pi}} \cos \frac{\theta}{2} \left(1 - 2\nu + \sin^2 \frac{\theta}{2}\right) \\
    u_y &= \frac{K}{\mu} \sqrt{\frac{r}{2\pi}} \sin \frac{\theta}{2} \left(2 - 2\nu + \cos^2 \frac{\theta}{2}\right)
\end{align*}
\] (3.27a) (3.27b)

where

\[ r = \sqrt{x^2 + y^2} \theta = \tan^{-1} \frac{y}{x} \] (3.28)

After the crack tip the surface is \( T = 0 \). In the cohesive zone, the constitutive relation for the normal traction \( T \) is taken from a potential \( \phi \) as \( T = \partial \phi / \partial \Delta \), where
\( \Delta \) is the displacement jump across the interface. The form of \( \phi \) is

\[
\phi = \phi_n + \phi_n \exp \left( -\frac{\Delta_n}{\delta_n} \right) \left\{ \left[ 1 - r + \frac{\Delta_n}{\delta_n} \right] \frac{1 - q}{r - 1} - \left[ q + \left( \frac{r - q}{r - 1} \right) \frac{\Delta_n}{\delta_n} \right] \exp \left( -\frac{\Delta^2_n}{\delta^2_t} \right) \right\}
\]

(3.29)

where \( \delta_n \) and \( \delta_t \) are the normal and tangential characteristic lengths, respectively, and the work of normal and tangential separation are

\[
\phi_n = e \sigma_{\text{max}} \delta_n, \quad \phi_t = \tau_{\text{max}} \delta_t \sqrt{\frac{\nu}{2}}
\]

(3.30)

where \( \sigma_{\text{max}} \) and \( \tau_{\text{max}} \) are the normal and shear cohesive strengths, respectively. The normal-shear coupling is included through parameters

\[
q = \frac{\phi_t}{\phi_n}, \quad r = \frac{\Delta^*_n}{\delta_n}
\]

(3.31)

where \( \Delta^*_n \) is the value of \( \Delta_n \) after a complete shear separation with \( T_n = 0 \). The characteristic lengths are taken to be \( \delta_n = 0.059 \text{ nm} \), and the interface strengths are \( \sigma_{\text{max}} = 7 \text{ GPa} \). In this case, the tangential effect is ignored by setting \( \delta_n = 0.059 \text{ m} \) and \( \tau_{\text{max}} = 0 \). So the fracture energy \( \Gamma_0 = \phi_n \) and \( \sigma_{\text{coh}} = \sigma_{\text{max}} \). Here we define at normalized parameter

\[
\tilde{K} = K/K_0
\]

(3.32)

where

\[
K_0 = \sqrt{\frac{ET_0}{1 - \nu^2}}
\]

(3.32)

The physical interpretation of \( \tilde{K} \) is that when the crack tip starts to propagate, \( \tilde{K} \) equals to 1. The model is loaded incrementally with a \( \dot{\tilde{K}} = 0.01, 100 \text{ s}^{-1} \) at 900 K. The toughness as crack position is plotted in Fig. 3.14. It is observed that toughness is changing as a function of strain rate. The step is the tip motion is due to prevention of dislocation in front of it. Dislocation configuration around the crack
3.4 Discussion and summary

In general, for the range of strain rates and temperatures considered in this study we found that the modified FIRE solver is capable of solving (2.1) in less than 500 iterations; the computational cost of each iteration is equivalent to that of a single regular DDD step. We also found that the computational efficiency is independent of the temperature and strain rate. Since the glide time scale has been eliminated, simulation of rate-controlled thermal processes over the entire range of parameters studied here can be achieved with the same amount of computational cost by scaling
3.4. DISCUSSION AND SUMMARY

Figure 3.15: Dislocation configuration at crack tip at $\dot{K}/K_0 = 2$ when $\dot{K} = 100$ s$^{-1}$ under 900 K. The contour plot shows the distribution of $\sigma_y$.

Due to the general nature of the model, other mechanisms and events can be included. For example the energy barrier can be modified to account for strain aging of obstacles during deformation, perhaps paving a way to incorporate negative rate sensitivity into DDD/TADD simulations. Diffusive climb can also be incorporated within our model, by including the solution of an auxiliary vacancy diffusion problem [1] at the appropriate time scale within our incremental scheme. Without the burden of glissile time scale, TADD is able to reach much longer time scale using real diffusivity and strain rates in experiments.
Diffusion assisted climb of dislocations is a non-conservative motion where the dislocation can climb out of its slip plane by absorbing and emitting vacancies. Climbing dislocations present a potent relaxation mechanism that prevents formation of large pileups by surmounting small obstacles. Given that climbing dislocations contribute significantly to creep, relaxation and other high temperature deformation modes. [102, 103, 104, 105], a thorough understanding of dislocation climb is extremely critical. Sophisticated models based on empirical observations of creep, exist, but the predictive power of these models for new material development is unclear. We now present a new model of dislocation climb that has has four essential components: a) computing the rate of climb of dislocations at arbitrary temporal scales, b) coupling of vacancy concentration fields between dislocations that are close together, c) solving a coupled mechanical-diffusion problem accurately and d) decoupling glide and climb time scales.
4.1 Climb of edge dislocations

The governing equation for diffusion in the volume excluding the dislocation core, is adequately described by stress driven diffusion equation [67]

\[ \frac{\partial c}{\partial t} = D_v \nabla^2 c + \frac{D_v \Omega}{kT} \nabla \cdot (c \nabla p) \text{ in } V \]  (4.1)

where \( c \) is the vacancy concentration, \( D_v \) is the diffusion coefficient of vacancy, \( k \) is the Boltzmann constant, \( \Omega \) is the atomic vacancy volume, \( T \) is temperature and \( p \) is local pressure.

The mechanical driving force for climb is the component of Peach-Koehler force (2.2) perpendicular to the glide plane of the dislocation [106]

\[ F^{cl} = \left[ (b \cdot \sigma) \times \zeta \right] \cdot \left( b \times \zeta \right) \left| b \times \zeta \right| \]  (4.2)

where \( \sigma \) is the local stress tensor, \( b \) is the Burgers vector of dislocation and \( \zeta \) is the unit vector along the dislocation line.

Osmotic force is associated with vacancy generation and destruction. Vacancies can be created or absorbed by the dislocation core. This causes extension or shrinkage of extra plane of atoms defining the dislocation and therefore the dislocation climbs. The variation of free energy change due to vacancies is described by the osmotic force, given by

\[ F_{os} = -\frac{kTb}{\Omega} \ln \left( \frac{c}{c_0} \right) \]  (4.3)

where \( c \) is the vacancy concentration, \( b \) is signed magnitude of Burgers vector and \( c_0 \) is the reference vacancy concentration at a given temperature \( T \).

Drag force arises when vacancies are accumulating/annihilating within in the vicinity of the dislocation core, under the influence of gradient of the pressure field.
the dislocation. The drag force is negligible compared with the other tow forces [67] and hence it is neglected. Ham [107] examined the stress-assisted climb of an edge dislocation and replaced the stress field by a cylinder with an effective capture radius. By an appropriate choice of capture radius $r_c$, the pressure driven term in (4.1) can be neglected. Therefore, the diffusion problem is coupled with mechanical problem through equilibrium concentration, where the climbing part of Peach-Koehler force in (4.2) is balanced by osmotic force (4.3). An equilibrium concentration corresponding to climb force $F^{cl}$ on dislocation is

$$c^{eq} = c_0 \exp \left( \frac{F^{cl} \Omega}{b k T} \right) \quad (4.4)$$

where $F^{cl}$ is the climbing part of Peach-Koehler force applied on dislocation and $b$ is the signed magnitude of Burgers vector. The climbing velocity of the dislocation $v^{cl}$ can be obtained from mass conservation as

$$v^{cl} b = \Omega \oint_{\partial C} J \cdot n ds = \Omega I$$

(4.5)

where $\partial C$ is a circle round dislocation capture region $C$ with capture radius $r_c$, $J$ is the flux and $I$ is the total vacancy current around $\partial C$. Therefore the problem of finding the climb rate of a dislocation is reduced to determining the vacancy current around the capture radius. To simplify the diffusion problem, the following assumptions are made:

(a) Drag force due to the local dislocation stress field pressure, last term in (4.1), is neglected outside the core region, resulting in a linear diffusion equation

$$\frac{\partial c}{\partial t} = D_v \nabla^2 c$$

(4.6)
The dislocation core region $C$ is represented as a line source/sink for vacancies. The vacancy concentration in the core region is assumed uniform $c^c$. Outside the core region follows diffusion equation (4.6).

Depending on jog formation energy, jog density and stacking fault energy, the dislocation is not always capable of maintaining the equilibrium concentration and the concentration at the core can be approximated by using a kinetic rate equation defined by a constant $K$. The reverse net from core to bulk $I'$ can be defined as

$$I' = 2\pi r_c K (c^{eq} - c^c)$$

(4.7)

The instantaneous flux at time $\bar{t}$ into the core region is given by

$$I = -2\pi r_c D_v \left[ \frac{\partial c}{\partial r} \right]_{r=r_c}$$

and the flux balance $I_i = I'_i$ is satisfied on the interface $\partial C$. In the next section, we will introduce the solution to this problem.

### 4.2 Dislocation climb in an infinite medium

Our discussion starts with the dislocation climb in infinite medium. First, we will provide a new expression for single dislocation climb. Then a dislocation ensemble is considered, emphasizing the climb rate coupling.

#### 4.2.1 Formulation for transient climb of dislocations in an infinite medium

Consider a single straight edge dislocation in an infinite medium subjected to a constant mechanical driving force. The time dependent radial concentration distribution
4.2. DISLOCATION CLIMB IN AN INFINITE MEDIUM

$c(r, t)$ in a region $r_c < r < \infty$ completely determines the climb rate of the dislocation. The initial conditions and boundary conditions are

$$c(r,0) = c^\infty, \ c(r_c,t) = c^c$$  \hspace{1cm} (4.8)

Several non-dimensional quantities can be defined to simplify our analysis. These are the non-dimensional length scale defined by $\bar{r} \equiv r/r_c$ and an non-dimensional time scale $\bar{t} \equiv D_v t/r_c^2$. The exact solution of this problem (4.6) and (4.8) is given by [55] and [56]. The flux at the surface $r = r_c$ can be expressed as

$$I = 2\pi D_v (c^c - c^\infty) G(\bar{t})$$  \hspace{1cm} (4.9)

where $G(\bar{t})$ is a non-dimensional flux. By the flux balance $I = I'$, (4.7) and (4.9), we can solve for $c^c$

$$c^c - c^\infty = \frac{c^{eq} - c^\infty}{1 + \bar{D}G(\bar{t})} \equiv \eta (c^{eq} - c^\infty)$$  \hspace{1cm} (4.10)

where $\bar{D}$ is non-dimensional kinetics parameter [1, 78] defined as

$$\bar{D} = \frac{D_v}{r_c K}$$  \hspace{1cm} (4.11)

and source efficiency

$$\eta = \frac{1}{1 + \bar{D}G(\bar{t})}$$  \hspace{1cm} (4.12)

When the transfer rate at core region is very high so that $\bar{D} \ll 1$, $c^c \approx c^{eq}, \eta \approx 1$ the kinetics is said to be diffusion-limited and when $\bar{D} \gg 1$, $c^c \approx c^\infty, \eta \approx 0$ the kinetics is source/sink-limited.

The exact solution to $G(\bar{t})$ is given either in terms of integrals or tabulated Bessel functions that are not readily usable. Perrochet [60] restated the boundary value problem (4.6) and (4.8) into a moving boundary in the region $r_c \leq r < R(t)$, shown
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Figure 4.1: Schematic of the boundary value problem of an edge dislocation climb in infinite media with the vacancy concentration \( c(r, t) \) maintains \( c^c \) on the core region boundary \( \partial C \) and \( c^\infty \) in far field. The radius of \( \partial C \) is \( r_c \) and the dashed line is the moving boundary \( R \) defined by (4.14)

in Fig. (4.1) such that \( c(r, 0) = c_0 \), \( c(r_c, t) = c^{eq} \), \( \frac{\partial c}{\partial r} (R, t) = 0 \). Perrochet [60] have then provided a high accuracy approximation for \( R(\bar{t}) \) and \( G(\bar{t}) \). From Perrochet [60] the non-dimensional flux \( G(\bar{t}) \) is given as

\[
G(\bar{t}) \approx \frac{1}{\ln \left(1 + \sqrt{\pi \bar{t}}\right)} \tag{4.13}
\]

\( \bar{R}(\bar{t}) \equiv \frac{R(\bar{t})}{r_c} \) can now be determined at any time \( \bar{t} \) by solving [60]

\[
\frac{\bar{R}^2}{\bar{R}^2 - 1} \ln \bar{R}^2 - 1 = 2 \ln \left(1 + \sqrt{\pi \bar{t}}\right) \tag{4.14}
\]

Using \( G(\bar{t}) \) the time dependent radial concentration distribution can be found to be
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\[
c(\vec{r}, \vec{t}) - c^\infty = \eta (c^{eq} - c^\infty) \left[ \frac{\ln \left( \frac{\vec{R}^2}{\vec{r}^2} \right) - 1 + \vec{r}^2/\vec{R}^2}{\ln \vec{R}^2 - 1 + 1/\vec{R}^2} \right]
\]  

(4.15)

Therefore, the dislocation climb rate is given by (4.5), (4.9) and (4.13)

\[
v_{cl} = \frac{\Omega I}{b} = \frac{2\pi D_v \Omega (c^{eq} - c^\infty)}{b \ln \left( 1 + \sqrt{\pi t} \right) + \tilde{D}}
\]  

(4.16)

and climb distance is given by integration the concentration profile at \( \tilde{t} \)

\[
s = \frac{-\Omega}{b} \int_{1}^{\tilde{R}(\tilde{t})} 2\pi \rho c(\vec{r}, \vec{R}) \, dr &= \frac{-\pi \rho^2 \Omega \left( c^{eq} - c^\infty \right)}{b} \left[ \frac{\tilde{R}^2 - 1}{4 \ln \left( 1 + \sqrt{\pi t} \right)} - 1 \right]
\]  

(4.17)

Now we will prove that these equations collapse to steady state solution when \( \tilde{t} \) and \( \tilde{R} \) are sufficiently large. Let \( c^\epsilon = c^{eq} \) and \( c^\infty = c_0 \). Since \( \left| 1 - \vec{r}^2/\vec{R}^2 \right| < 1 \) and \( \left| 1 - 1/\vec{R}^2 \right| < 1 \) and \( \ln \tilde{R} \approx \ln \left( 1 + \sqrt{\pi t} \right) \) by (4.14), then (4.15) and (4.16) becomes

\[
c(\vec{r}, \tilde{t}) - c_0 \approx (c^{eq} - c_0) \frac{\ln \left( \frac{\tilde{R}^2}{\vec{r}^2} \right)}{\ln \vec{R}^2}, \quad v_{cl} \approx \frac{2\pi D_v \Omega (c^{eq} - c_0)}{b \ln \tilde{R}}
\]  

(4.18)

which is the same as solution given by [106]. For a single dislocation climbing in infinite media, \( \tilde{R} \) will keep expanding in space at each instantaneous time and there is no steady-state solution. Or in other words the dislocation velocity and the concentration distributions will vary in time. However, since \( \ln \tilde{R} \) varies very slowly with increasing \( \tilde{R} \), (4.18) is considered as a steady state solution. The high accuracy closed form solution for the transient climb of a straight edge dislocation in infinite media is the first main result of this chapter.
Consider a single edge dislocation at origin at \( t = 0 \), subjected to a remote tensile stress \( \sigma_x \). Here we define the following non-dimensional terms:

\[
\bar{x} = \frac{x}{r_c}, \quad \bar{y} = \frac{y}{r_c}, \quad \bar{t} = \frac{D_v t}{r_c^2}, \quad \bar{V} = -\frac{v^{cl} r_c}{D_v}, \quad \bar{s} = -\frac{s}{r_c}, \quad \bar{\sigma} = \frac{F^{cl} \Omega}{b k T}
\]

(4.19)

where \((\bar{x}, \bar{y})\) is non-dimensional coordinate, \( \bar{t} \) is non-dimensional time, \( \bar{V} \) is non-dimensional climb velocity, \( \bar{s} \) is non-dimensional climb distance and \( \bar{\sigma} \) is non-dimensional applied stress. For demonstration purposes the material is chosen as Aluminum with Young’s modulus \( E \) is 70 GPa, shear modulus \( \mu \) is 26.2 GPa, Poisson’s ratio \( \nu \) is 0.33, the magnitude of Burgers vector \( b \) is 0.25 nm and the atomic vacancy volume \( \Omega \) is \( 1.661 \times 10^{-11} \text{nm}^3 \). Unless otherwise mentioned the temperature is kept constant at 823 K. The corresponding reference concentration \( c_0 \) is \( 4.127 \times 10^6 \mu \text{m}^{-3} \) and vacancy diffusivity \( D_v \) is \( 3.198 \times 10^{-9} \text{m}^2/\text{s} \) [65, 108]. The non-dimensional climb stress on the dislocation \( \bar{\sigma} \) is 0.1. Therefore by (4.4) the equilibrium concentration \( c^{eq} \) is \( 4.561 \times 10^6 \mu \text{m}^{-3} \). Also we choose \( \bar{D} = 0.1 \) to represent a mix state of diffusion-limited and source-limited case. Figure 4.2(a) shows the non-dimensional climb velocity \( \bar{V} \) plotted versus the non-dimensional time \( \bar{t} \) with \( r_c = 10b \). The solid line represents the analytical solution of (4.16) and the dashed lines the numerical results obtained from an implementation of the discrete dislocation (DD) formulation from [1]. The DD solution was obtained by a numerical integration scheme of instantaneous sources given with the time step \( d\bar{t} = 0.2 \), which is the largest time step to insure the convergence shown Appendix B. Figure 4.2(b) shows the concentration distributions for various times once again obtained from the analytical solution of (4.15) (solid lines) and the numerical DD solution (dashed lines) for various values of time. The concentration distribution obtained from the analytical formulation and DD are almost indistinguishable. The climb velocity predicted by the analytical result is lower than the DD because in their formulation Ayas et al. [1] have introduced...
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![Figure 4.2: A single edge dislocation in infinite medium under applied stress $\bar{\sigma} = 0.1$: (a) The normalized time $\bar{t}$ versus normalized climb rate $\bar{V}$, solid line is (4.16) and dashed line result from [1], the inset shows the schematic of single edge dislocation climbing in infinite medium; (b) The normalized concentration distribution at different time $\bar{t}$ with $\bar{y}$ adjacent with dislocation, solid line is (4.15) and dashed line is the result from [1].]

a time shift to remove singularity in the instantaneous source solution. Since the inherent singularity is accounted by the analytical time integration in our continuous source formulation (4.13) is applicable for a wide range of time [60], no further numerical treatment is needed. The numerical validation of climb of single edge dislocation is the second main result of this chapter.

4.2.2 Dislocation ensembles: A superposition framework

Consider two or more dislocations in the infinite medium as shown in Fig. 4.3 with a global coordinate $\mathbf{x} = (x, y)$, shown in Fig. 4.3. Assuming a constant background concentration $c(\mathbf{x}, t) = c^\infty$ and a constant mechanical driving force, we are interested
in solving for the unknown concentration distribution and its evolution in time. At
time \( t \), each dislocation \( i \) has position \( \mathbf{x}_i = (x_i, y_i) \) and radius \( r_c \) and created at time \( t_i < t \). We extend the solution in the previous section to ensembles by using the
linearity of (4.6) and using a superposition scheme to determine the concentration
distribution for multiple dislocations.

The concentration profile for a each dislocation can now be rewritten in a more
convenient form from (4.15) such that

\[
c_i(\mathbf{x}, t) = c_i^* f \left( \tilde{r}_i, \bar{R}_i \right) \tag{4.20}
\]

where \( \tilde{r}_i = |\mathbf{x} - \mathbf{x}_i|/r_c \) is the normalized distance to the dislocation \( i \), \( c_i^* \) is the
concentration at the capture radius \( \tilde{r} = 1, \bar{R}_i \) is the influence radius at time \( \bar{t}_i = (t - t_i)/r_c \)
defined by (4.14) and \( f(\tilde{r}, \bar{R}) \) is the spatial distribution of concentration

\[
f \left( \tilde{r}, \bar{R} \right) = \begin{cases} 
\frac{\ln(\bar{R}^2/\tilde{r}^2) - 1 + \tilde{r}^2/\bar{R}^2}{\ln(\bar{R}^2) - 1 + 1/\bar{R}^2} & 1 \leq r \leq \bar{R} \\
0 & \text{otherwise}
\end{cases} \tag{4.21}
\]

In order to explain the coupling process, consider 2 dislocations that were created
at the same instant in time. At this instant the concentration profiles at every location
in the body will be the simple sum of contributions from each dislocation. As time
evolves the sphere of influence of each dislocation grows, (growth in \( \bar{R}_i \)). When \( \bar{R}_i \)
encompasses the other dislocation, the concentration at the boundary \( \tilde{r}_i = 1 \) will
no longer be equal to \( c_i^{eq} - c^\infty \), but will be a function of time and coupled with the
concentration field of the other dislocation. In order to rigorously create a framework
for coupling concentrations between dislocations, we can see that the concentration
at dislocation \( i \) consists of three parts: the self-contribution \( c_i^* \), contribution from all
other source \( \sum_{j=1,j \neq i}^{n} c_j^* f \left( \tilde{r}_{ij}, \bar{R}_j \right) \) with distance \( \tilde{r}_{ij} = |\mathbf{x}_i - \mathbf{x}_j|/r_c \) and the background
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Figure 4.3: Decomposition of dislocation $i$ and $j$ with distance $r_{ij}$ climbing in infinite medium into continuous source field $c_i$, $c_j$ and the constant $c^\infty$. In source filed $c_i$ is characterized with source strength $c^\star$ and moving boundary $R_i$ by (4.20) and (4.21). The description applies to source filed $c_j$ concentration $c^\infty$, shown in Fig. 4.3(b). Considering the condition $c_i \left( x_i, \tilde{t} \right) = c^\star_i$ that the concentration equals to equilibrium concentration at the dislocation position, we have

$$c^\star_i + \sum_{j=1, j\neq i}^n c^\star_j f \left( \tilde{r}_{ij}, \tilde{R}_j \right) = c^e_i, \ (i = 1...n) \quad (4.22)$$

By (A.4) and (A.11), the instantaneous flux into the core region is

$$I_i \left( \tilde{t}_i \right) = I^\text{self}_i + I^\text{other}_i = \frac{2\pi D c^\star_i}{\ln \left( 1 + \sqrt{\pi \tilde{t}_i} \right)} + \sum_{j=1, j\neq i}^n \frac{4\pi D_v c^\star_j}{R^2_j \ln R^2_j - R^2_j + 1} \quad (4.23)$$

By the flux balance $I_i = I^\prime_i$ at the interface, putting (4.23) and (4.7) together and solving for $c^e$, we have

$$c^e_i = c^\star_i - \frac{\tilde{D}}{\ln \left( 1 + \sqrt{\pi \tilde{r}} \right)} c^\star_i - \sum_{j=1, j\neq i}^n \frac{2\tilde{D}}{R^2_j \ln R^2_j - R^2_j + 1} c^\star_j \quad (4.24)$$

Substituting (4.24) into constraints (4.22), we have the modified equations

$$h \left( \tilde{t}_i \right) c^\star_i + \sum_{j=1, j\neq i}^n c^\star_j f \left( \tilde{r}_{ij}, \tilde{R}_j \right) = c^\star_i - c^\infty, \ (i = 1...n) \quad (4.25)$$
4.2. DISLOCATION CLIMB IN AN INFINITE MEDIUM

with the definition

\[ h(t) = 1 + \frac{\bar{D}}{\ln \left(1 + \sqrt{\pi t}\right)} \]  

(4.26)

\[ f(r, R) = \begin{cases} \ln \left(\frac{R^2}{r^2}\right) - 1 + \frac{(r^2 + 2\bar{D})/R^2}{\ln(R^2) - 1 + 1/R^2} & 1 \leq r \leq R \\ 0 & \text{other} \end{cases} \]  

(4.27)

So (4.25) can be written in matrix form

\[
[F] [C^*] = [C^{eq}] - c^\infty
\]  

(4.28)

where \([F]\) is the coupling matrix

\[
[F] = \begin{bmatrix}
h_1 & f_{12} & f_{13} & \cdots & f_{1n} \\
f_{21} & h_2 & f_{23} & \cdots & f_{2n} \\
f_{31} & f_{32} & h_3 & \cdots & f_{3n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
f_{n1} & f_{n2} & f_{n3} & \cdots & h_n
\end{bmatrix}, h_i \equiv h(t_i), f_{ij} \equiv f(\bar{r}_{ij}, \bar{R}_j) \]  

(4.29)

\([C^*]\) is the unknown source strength

\[
[C^*] \equiv \begin{bmatrix} c_1^* & c_2^* & c_3^* & \cdots & c_n^* \end{bmatrix}^T
\]  

(4.30)

and \([C^{eq}]\) is the equilibrium concentration

\[
[C^{eq}] \equiv \begin{bmatrix} c_1^{eq} & c_2^{eq} & c_3^{eq} & \cdots & c_n^{eq} \end{bmatrix}^T
\]  

(4.31)
Equation (4.28) can be solved for the unknown concentrations at each dislocation \( c_i^* \). The coefficients of the coupling matrix \( f_{ij} \) represents the concentration contribution at dislocation \( i \) by dislocation \( j \). Combining (4.5) and (4.23), the climb rate \( v_{ci}^\text{cl} \) is

\[
v_{ci}^\text{cl} (\bar{t}_i) = \frac{\Omega I_i (\bar{t}_i)}{b_i} = \frac{\Omega}{b_i} \left[ \frac{2\pi D_c c_i^*}{\ln \left( 1 + \sqrt{\pi I_i} \right)} + \sum_{j=1, j\neq i}^{n} \frac{4\pi D_c c_j^*}{R_j^2 \ln R_j^2 - R_j^2 + 1} \right]
\] (4.32)

The total concentration at any location in the body can now be simply written as the sum of the contributions from each dislocation as

\[
c (x, \bar{t}) = \sum_{i=1}^{n} c_i^* f (\bar{r}_i, \bar{R}_i) + c^\infty
\] (4.33)

with \( \bar{r}_i = |x - x_i|/r_c \). Therefore, solving for the unknown time dependent concentration for a dislocation ensemble for arbitrary values of time in (4.22) to accommodate dislocation coupling is the third main result of this chapter. Equation (4.28) is reminiscent of Gu et. al.’s [76] approach albeit in steady state.

### 4.2.3 A analytic solution of two positive edge dislocation climb in infinite medium

In order to illustrate our formulation, we employ it to study two positive edge dislocations in an infinite medium. The two dislocations are initiated at the same time and are under the influence of a constant driving force, \( F^\text{cl} / b \). The first application is that of two positive edge dislocations, 1 and 2, with initial spacing \( L \) under the constant stress \( \sigma_x \). Since the shear stress on each dislocation is zero, the dislocation spacing will not change. Also since dislocation is created at the same time, then \( \bar{t}_1 = \bar{t}_2 = \bar{t} \)
and $\bar{R}_1 = \bar{R}_2 = \bar{R}$. Define normalized spacing $\bar{L} = L/r_c$ and substitute $\bar{r}_{12} = \bar{r}_{21} = \bar{L}$ into (4.28), we have the source strength

$$c_1^* = c_2^* = \frac{1}{h(\bar{t}) + f(\bar{L}, \bar{R})}$$

Substitute into (4.32), we have the climb rate for of each dislocation after $\bar{R} > \bar{L}$, then we have

$$v_{12}^{cl} = \begin{cases} \frac{2\pi D_c \Omega (c^q - c^\infty)/b}{\ln(1 + \sqrt{\pi} \bar{t}) + D} & \bar{R} \leq \bar{L} \\ \frac{2\pi D_c \Omega (c^q - c^\infty)/b}{2 \ln \bar{R} - \ln \bar{L} - 1 + (\bar{L}^2 + 1)/2R^2 + D} & \bar{R} > \bar{L} \end{cases}$$

All other input parameters remain the same as the single dislocation case. Equation (4.35) is plotted as non-dimensional time $\bar{t}$ and climb velocity $\bar{V}$ in Fig. 4.4(a). When $\bar{t}$ is small each dislocation is climbing independently just like the single dislocation climb (4.16) and climb rate is local. However, when one dislocation is under the concentration of the other, the climb rate will become non-local. Fig. 4.4(b) shows the normalized concentration distribution at different time when $\bar{L} = 100$ with $\bar{y}$ adjacent with dislocation. We can see the the concentration coupling develops as time goes on.

### 4.2.4 A steady state approximation

When the time is sufficiently large and the circle of influence of each dislocation $R_i(t)$ is larger than maximum dislocation spacing, the vacancy concentration is independent of time (steady state). We have proven for a single dislocation climb that our model collapses to the steady state solution for large times in Section 4.2.1. Here we will provide the framework for dislocation ensembles. By the superposition scheme in
Figure 4.4: (a) The normalized time $\bar{t}$ versus normalized climb rate $\bar{V}$ when $\bar{\sigma} = 0.1$ for two edge dislocations in infinite medium, solid line is (4.35) and dash line is (4.16), the inset shows the schematic of two edge dislocations climbing in infinite medium; (b) The normalized concentration distribution at different time when $\bar{L} = 100$ with $\bar{y}$ adjacent with dislocation.
(4.22), we have

\[
c_i^* + \sum_{j=1,j\neq i}^n \frac{\ln \left( \bar{R}/\bar{r}_{ij} \right)}{\ln R} c_j^* + c^\infty = c_i^{eq}, \quad (i = 1...n)
\]  

(4.36)

where \( \bar{R} = R^\infty/r_c \). Denoting \( f_{ij}^{st} = \ln \left( \bar{R}/\bar{r}_{ij} \right) / \ln \bar{R} \), equation (4.36) can be written in matrix form

\[
\begin{bmatrix}
1 & f_{12}^{st} & f_{13}^{st} & \cdots & f_{1n}^{st} \\
1 & f_{23}^{st} & f_{24}^{st} & \cdots & f_{2n}^{st} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\text{sym} & \ddots & \ddots & \ddots & 1
\end{bmatrix}
\begin{bmatrix}
c_1^* \\
c_2^* \\
\vdots \\
c_n^*
\end{bmatrix} =
\begin{bmatrix}
c_1^{eq} \\
c_2^{eq} \\
\vdots \\
c_n^{eq}
\end{bmatrix} - c^\infty
\]

(4.37)

Solving for \( c_i^* \) and substituting into (4.18) to get the contraction profile

\[
c(x) = \sum_{i=1}^n c_i^* \frac{\ln \left( \bar{R}/\bar{r}_i \right)}{\ln R} + c^\infty
\]

with \( \bar{r} = |x - x_i|/r_c \). By (4.5) and (A.5), the climb velocity is

\[
v_i^{cl} = -\frac{\Omega I_i^{st}}{b_i} = -\frac{2\pi D_v \Omega c_i^*}{b_i \ln \bar{R}}
\]

(4.38)

A recently work by Gu et al. [76] provides a steady state framework for 3d DDD dislocation climb which considers the climb coupling through Green’s function. The coupling in 2D can be expressed as follows

\[
-\frac{b_i v_i^{cl}}{4\pi D_v \Omega} \int_{-\infty}^{\infty} \frac{dz}{\sqrt{z^2 + r_c^2}} - \sum_{j=1,j\neq i}^n \frac{b_j v_j^{cl}}{4\pi D_v \Omega} \frac{dz}{\sqrt{z^2 + r_{ij}^2}} = c_i^{eq} - c^\infty
\]

(4.39)
With an outer cut-off of $R^\infty \gg r_c$ and $R^\infty \gg r_{ij}$ in the integral and the integral $\int_{-R^\infty}^{R^\infty} \left( \frac{1}{\sqrt{z^2 + r_c^2}} \right) dz = \ln \left( \frac{\sqrt{(R^\infty)^2 + r_c^2 + R^\infty}}{\sqrt{(R^\infty)^2 + r_c^2 - R^\infty}} \right) \approx 2 \ln \left( \frac{R^\infty}{r_c} \right)$ \[76\]. By the same procedure, we can obtain $\int_{-R^\infty}^{R^\infty} \left( \frac{1}{\sqrt{z^2 + r_{ij}^2}} \right) dz \approx 2 \ln \left( \frac{R^\infty}{r_{ij}} \right)$. Therefore, (4.39) becomes

$$\left( -\frac{b_i}{2\pi D_v \Omega} \ln \frac{R^\infty}{r_c} \right) v_i^{cl} + \sum_{j=1,j\neq i}^{n} \left( -\frac{b_j}{2\pi D_v \Omega} \ln \frac{R^\infty}{r_{ij}} \right) v_j^{cl} = c_i^q - c^\infty$$ \hspace{1cm} (4.40)

Now substituting (4.38) into (4.36) and rearranging terms, we have

$$\left( -\frac{b_i}{2\pi D_v \Omega} \ln \frac{R^\infty}{r_c} \right) v_i^{cl} + \sum_{j=1,j\neq i}^{n} \left( -\frac{b_j}{2\pi D_v \Omega} \ln \frac{R^\infty}{r_{ij}} \right) v_j^{cl} = c_i^q - c^\infty$$

which is the same as (4.40). Therefore, we prove that the steady state approximation (4.37) and (4.38) is equivalent to Gu’s method [76] in 2d under diffusion-limited case.

### 4.3 Dislocation climb in finite body

We will consider the effect of finite body and restate the framework on the superposition principle.

#### 4.3.1 A transient framework

Considering a finite body with dislocations inside, shown in Fig. 4.5(a), the boundary value problem is the governing equation (4.6) in $V$ with the boundary condition

$$c = c_0 \text{ on } B_c$$

$$J \cdot n = J_0 \text{ on } B_J$$

$$c(x_i) = c_i^e \text{ on } \Gamma_i$$

$$c = c_0 \text{ on } B_c$$

$$J \cdot n = J_0 \text{ on } B_J$$

$$c(x_i) = c_i^e \text{ on } \Gamma_i$$

(4.41a) \hspace{1cm} (4.41b) \hspace{1cm} (4.41c)
4.3. DISLOCATION CLIMB IN FINITE BODY

where $B_c$ is the prescribed concentration boundary, $B_J$ is the prescribed flux boundary and $\Gamma_i$ is the inter core boundary of dislocation $i$ located at $x_i$ with radius of $r_c$. $c^c_i$ is the concentration at $\Gamma_i$. The vacancy concentration is written as the superposition of two fields

\[ c = \tilde{c} + \hat{c}; \quad \mathbf{J} = \hat{\mathbf{J}} + \tilde{\mathbf{J}} \text{ in } V \]  

as illustrated in Fig. 4.5. The $\tilde{\text{\~{}c}}$ field is the sum of concentration profile of $n$ continuous source $\tilde{c}_i$ ($i = 1..n$) in homogeneous infinite medium associated with each dislocation $\tilde{c} = \sum_{i=1}^{n} \tilde{c}_i$. The each source $i$ maintains a constant concentration $c^*_i$ on the inner boundary $\Gamma_i$. The governing equation for $\tilde{c}$ field is

\[ \frac{\partial \tilde{c}}{\partial t} = D_v \nabla^2 \tilde{c} \]  

with the boundary values at the boundary

\[ \tilde{c} = \tilde{c}^B_c \text{ on } B_c; \quad \hat{\mathbf{J}} = \hat{\mathbf{J}}^B_J \text{ on } B_J \]  

The $\tilde{\text{\~{}c}}$ field is to correct for the original boundary condition (4.41). The governing equation of $\hat{c}$ field is

\[ \frac{\partial \hat{c}}{\partial t} = D_v \nabla^2 \hat{c} \]  

with the boundary values at the boundary

\[ \hat{c} = c_0 - \tilde{c}^B_c \text{ on } B_c; \quad \hat{\mathbf{J}} = \hat{\mathbf{J}}^B_J \text{ on } B_J \]  

Since the governing equation (4.6) is linear. After solving $\tilde{c}$ field and $\hat{c}$ field respectively, the superposition scheme (4.42) gives the solution to BVP (4.6) and (4.41).
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The field is solved by finite element method. The field is solved by the similar method in Section 4.2.2 but replacing $c^\infty$ with local concentration from $\tilde{c}$ field,

$$c^*_i + \sum_{j=1,j\neq i}^{n} c^*_j g(\vec{r}_{ij}, \vec{R}_j) = c^*_i - \hat{c}(\vec{x}_i), \ (i = 1...n) \tag{4.47}$$

By (A.4), (A.11) and (A.14), the total flux $I_i$ into the core region at dislocation $i$ is

$$I_i(t_i) = I_i^{\text{self}} + I_i^{\text{other}} + I_i^{\text{back}} = \frac{2\pi D_v c^*_i}{\ln \left(1 + \sqrt{\frac{\pi}{\pi t_i}} \right)} + \sum_{j=1,j\neq i}^{n} \frac{4\pi D_v c^*_j}{\bar{R}_j^2 \ln \bar{R}_j^2 - \bar{R}_j^2 + 1} + \frac{\pi r_c}{2} \frac{\partial \tilde{c}(\vec{x}_i)}{\partial t} \tag{4.48}$$

Considering the flux out of the core region and flowing the same procedure of Section 4.2.2, we have

$$c^c_i = c^e_i - \frac{\bar{D}}{\ln \left(1 + \sqrt{\frac{\pi}{\pi t_i}} \right)} c^*_i - \sum_{j=1,j\neq i}^{n} \frac{2\bar{D}}{R_j^2 \ln \bar{R}_j^2 - \bar{R}_j^2 + 1} c_j^* - \frac{\bar{D}}{2} \hat{c}(\vec{x}_i) \tag{4.49}$$

where $\frac{\partial \tilde{c}(\vec{x}_i)}{\partial t} = \frac{D_v}{r_c^2} \hat{c}(\vec{x}_i)$. Then substituting into (4.47), we have

$$h(t_i) c^*_i + \sum_{j=1,j\neq i}^{n} c^*_j f(\vec{r}_{ij}, \bar{R}_j) = c^e_i - \hat{c}(\vec{x}_i) - \frac{\bar{D}}{2} \hat{c}(\vec{x}_i) \tag{4.50}$$

By the same notation in (4.29), the matrix form of (4.50) can be written as

$$\begin{bmatrix} h_1 & f_{12} & f_{13} & \cdots & f_{1n} \\ f_{21} & h_2 & f_{23} & \cdots & f_{2n} \\ f_{31} & f_{32} & h_3 & \cdots & f_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ f_{n1} & f_{n2} & f_{n3} & \cdots & h_n \end{bmatrix} \begin{bmatrix} c^*_1 \\ c^*_2 \\ c^*_3 \\ \vdots \\ c^*_n \end{bmatrix} = \begin{bmatrix} c^e_1 \\ c^e_2 \\ c^e_3 \\ \vdots \\ c^e_n \end{bmatrix} - \begin{bmatrix} \hat{c}(\vec{x}_1) \\ \hat{c}(\vec{x}_2) \\ \hat{c}(\vec{x}_3) \\ \vdots \\ \hat{c}(\vec{x}_n) \end{bmatrix} - \frac{\bar{D}}{2} \begin{bmatrix} \hat{c}(\vec{x}_1) \\ \hat{c}(\vec{x}_2) \\ \hat{c}(\vec{x}_3) \\ \vdots \\ \hat{c}(\vec{x}_n) \end{bmatrix} \tag{4.51}$$
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Figure 4.5: Decomposition of the transient diffusion problem with \( n \) dislocations climbing within a finite body into \( n \) homogeneous infinite field \( \tilde{c}_i \) \((i = 1..n)\) containing one continuous source with strength \( c_i^* \) and a complementary problem \((\tilde{c})\) without sources that enforced the boundary conditions

After solving \( c_i^* \), the corresponding climb rate \( v_i^{cl} \) and concentration profile \( c \) can be obtained by (4.32) and (4.33), respectively.

### 4.3.2 Steady state case

A steady state problem of finite body is expressed in \( \nabla^2 c = 0 \) in \( V \) with the boundary condition

\[
c = c_0 \text{ on } B_c
\]  
(4.52a)

\[
J \cdot n = J_0 \text{ on } B_J
\]  
(4.52b)

\[
c(x_i) = c_i^e \text{ on } \Gamma_i
\]  
(4.52c)

Using superposition scheme, the BVP of \( \sim \) field is

\[
\nabla^2 \tilde{c} = 0
\]  
(4.53a)

\[
\tilde{c} = \tilde{c}^{B_c} \text{ on } B_c; \quad \tilde{J} = \tilde{J}^{B_J} \text{ on } B_J
\]  
(4.53b)
and the BVP of $\sim$ field is

\[
\nabla^2 \hat{c} = 0 \quad (4.54a)
\]
\[
\hat{c} = c_0 - \hat{c}^{B_c} \text{ on } B_c; \quad \hat{J} = J_0 - \hat{J}^{B_J} \text{ on } B_J
\]

(4.54b).

The $\sim$ field (4.54) is solved by finite element method. The $\sim$ field (4.53) is solved by the similar method in Section 4.2.4. Notice that $\hat{c}(x)$ is a function of $c^*_i$ ($i = 1..n$) due to the uniqueness of the solution to the steady state problem, which can be regarded as the feedback of $c^*_i$. Therefore, in order to maintain the boundary condition, we have

\[
\left(1 + \frac{\bar{D}}{\ln \bar{R}}\right)c^*_i + \sum_{j=1,j\neq i}^{n} \frac{\ln(\bar{R}/\bar{r}_{ij})}{\ln \bar{R}} c^*_j = c^e_i - \hat{c}(x_i, C^*)
\]

(4.55)

where

\[
[C^*] \equiv \begin{bmatrix} c^*_1 & c^*_2 & c^*_3 & \cdots & c^*_n \end{bmatrix}^T
\]

(4.56)

Denoting that

\[
[F^{st}] = \begin{bmatrix}
    h & f^{st}_{12} & f^{st}_{13} & \cdots & f^{st}_{1n} \\
    h & f^{st}_{23} & \cdots & f^{st}_{2n} \\
    h & \cdots & f^{st}_{3n} \\
    \text{sym} & \ddots & \vdots \\
    \vdots & \ddots & h
\end{bmatrix}
\]

(4.57)

and

\[
[H(C^*)] = \begin{bmatrix} \hat{c}(x_1, C^*) & \hat{c}(x_2, C^*) & \hat{c}(x_3, C^*) & \cdots & \hat{c}(x_n, C^*) \end{bmatrix}^T
\]

(4.58)

then (4.55) can rewritten as $[F^{st}] [C^*] = [C^e] - [H(C^*)]$ which defines an iterative scheme to solve $[C^*]$ when all the dislocations remain stationary:
4.4. NUMERICAL EXAMPLES AND DISCUSSION

1. For $j = 0$, initialize $[C^0]$ by the last converged solution and tolerance $\varepsilon$

2. At step $j$, calculate $[C^{j+1}] = [F^{st}]^{-1} \{[C^{eq}] - [H(C^j)]\}$

3. Stop when $|[C^{j+1}] - [C^j]| \leq \varepsilon$ and $[C^*] = [C^{j+1}]$; otherwise, $j = j + 1$ and go to 2.

4.4 Numerical examples and discussion

4.4.1 Single stationary dislocation in finite body

Consider a single dislocation located at in the center of a circle with radius $L$, shown in Fig. 4.6. $\tilde{L} = 200$ where $\tilde{L} = L/r_c$. The body is subject to tensile stress $\sigma_x$. The boundary condition is such that the concentration remains as $c^{eq}$ within $r_c$ and $c_0$ on the entire boundary. We fix the dislocation from climbing but calculate the climb anyway. This scenario corresponds to a dislocation that remains in the center of the control volume in both the steady state solution [106] and the transient solution [60]. Also we temperately disable the effect of the image force. The time step is chosen as $d\tilde{t} = 200$ to make sure $\tilde{R} < \tilde{L}$ in the first step.

Figure 4.6(a) shows the normalized time $\tilde{t}$ versus climb rate $\tilde{V}$. We can see that the climb rate follows the transient solution (4.16) initially and then it trends to the steady state solution. This is because the dislocation operates as a continuous source before the $\tilde{R}$ reaches the boundary. After that due to boundary condition, $\tilde{c}$ creates negative feedback which gradually establishes a constant climb rate. As we expected, in the long run the concentration response recovers the steady state solution. One essential feature of our algorithm is that we can predict the transient time form time dependent solution to steady state solution as function of sample size $\tilde{L}$, shown in Fig. 4.6(b). Here we chose $\tilde{L} = 50, 100, 200, 400$ and $800$. As $\tilde{L}$ increases, the
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Figure 4.6: (a) The normalized climb rate $\bar{V}$ as a function of normalized time $\bar{t}$ when a single edge dislocation fixed in the center of a square body with a radius $\bar{L}$ subject to a tensile stress $\sigma_x$. The dashed line is transient solution (4.16) and the dash-dot line is the steady state solution when $\bar{R} = \bar{L}$ in (4.18). (b) $\bar{V}$ as a function of $\bar{t}$ when a single edge dislocation climb within a square body for a range of $\bar{L}$. The dash line is the steady state solution (4.18). The image force is ignored.

required time scale is increased and the error between numerical result and steady state solution is decreased.

Now for the four choices of $\bar{L}$, we let the dislocation climb while maintain all other inputs are the same as last section. Figure 4.6(b) is the time-climb rate curve. The curve can be divided into three stages. The preliminary stage, where the dislocation behaves similar to the stationary case: start with a transient and approach the steady state climb velocity after $\bar{R} > \bar{L}$. When dislocation is close to the boundary, the interaction between the dislocation and the boundary keeps increasing. So the climb rate increases exponentially until it is absorbed by the boundary. Therefore, our
4.4. NUMERICAL EXAMPLES AND DISCUSSION

Figure 4.7: The normalized concentration profile $c/c_0$ and dislocation position at different time $\bar{t}$ for an applied stress $\bar{\sigma} = 0.1$ in body with radius $\bar{L} = 50$. The dislocation initially in the center and eventually climbs out of the body. The image force is ignored.

Figure 4.8: Schematic of a dislocation loop with radius $R_L$ shrinking by climb in a thin film of thickness $2d$.

methodology captures the two transients: from time dependent climb to steady state response and the acceleration due to the boundary.

4.4.2 Dislocation shrinkage in thin film

In this section we examine the annealing rate of a single prismatic loop located near the center of a thin film in Aluminum. As in Fig. 4.8, the loop is taken as an effective torus of large radius $R_L$, with much smaller core radius $r_c$. The film thickness is $2d$. The vacancy concentration is maintained at $c_0$. 
4.5. 

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Figure 4.9: For film thickness $\bar{d}=40, 80, 160$ and $\infty$, (a) the normalized loop shrinkage rate $\bar{V}$ as a function of normalized time $\bar{t}$ and (b) the normalized loop radius $\bar{R}_L$ as a function of time $\bar{t}$.

In this case we consider image force. As dislocations approach each other, new source is added to after each climb to account for the $\Delta c^{eq}$. We chose $R_L = 4r_c$ and chose four different $\bar{d} = d/r_c$ as 40, 80, 160 and $\infty$. Figure 4.9(a) measures the normalized loop shrinkage rate $\bar{V}$ as a function of normalized time $\bar{t}$. For each $\bar{d}$, it has the three stages similar with Fig. 4.6(b). We can see as $\bar{d}$ increases, the $\bar{t} - \bar{V}$ curve trends to shrinkage in infinite medium. Figure 4.6(b) measures the normalized loop radius $\bar{R}_L$ as a function of time $\bar{t}$.

### 4.5 Cooperation of thermal activation and climb

#### 4.5.1 Thermal activation revisit

In Section 3.3.1 we have examined the yielding stress when the first dislocation is thermally activated over an obstacle. Now we will find the yielding stress when the...
first dislocation climbs over the obstacle. A pileup is loaded with constant strain rate on 45 degree slip plane in infinite medium, shown in Fig. 4.10. The input parameter is $L_{\text{obs}} = 0.2 \ \mu m$, $\tau_s = 50 \ \text{MPa}$ and $\tau_{\text{obs}} = 800 \ \text{MPa}$. The athermal yielding stress $\tau_Y$ is given by (2.7). The relation between the strain rate and yielding stress in thermal activation is shown in Fig. 4.11(a). The horizontal axis is strain rate and the vertical axis is the yielding for certain strain rate and temperature normalized by $\tau_Y$. Again, Fig. 4.11(a) shows thermal effect and a minor rate effect. Now for the same condition as thermal activation, yielding stress is defined as applied stress when the first dislocation climbs over the obstacle. The yielding stress as a function of strain rate is shown in Fig. 4.11(b). In the high strain rate range or in the low temperature range, the dislocation escapes thermally. This is because the applied stress reaches to $\tau_Y$ much earlier than dislocation accumulates sufficient amount of vacancies for it to climb. In the high temperature and low strain rate range, where the climb happens most freely, a large rate effect occurs.

If we superpose Fig. 4.11(a) on Fig. 4.11(b), we will see the competition between thermal activation and climb, as shown in Fig. 4.12. We can see a transient region which divides thermal activation region and climb region. For given strain range, as the temperate decreases the transient region moves towards the low strain rate
4.5. COOPERATION OF THERMAL ACTIVATION AND CLIMB

Figure 4.11: Strain rate vs. yielding stress curve under (a) thermal activation and (b) diffusion-assisted climb, showing different rate sensitivity.

side. Eventually, below a critical temperature, the entire strain range becomes by thermal activation only. We can see that dislocation climb is dominant in the high temperature, low strain rate. Consequently, we can infer that high temperature creep would be dominant by climb mechanism while thermal activation is dominant in the rest of the strain rate and temperature range.

Also in each temperature of Fig. 4.12, we can determine a transition strain rate which is on the boundary across the thermal activation region and climb region. This transition strain rate increases as temperature goes up, showing the kinetic due to different mechanisms changes as a function of temperature.

4.5.2 Creep of single crystal for multi-slip

A rectangular sample of 6 $\mu$m $\times$ 1 $\mu$m is studied with multiple sources and obstacles on multiple slip systems, shown in Fig. 4.13. The elastic modulus is $E = 70$ GPa, Poisson’s ratio is $\nu = 0.33$ and the magnitude of Burgers vector $b = 0.25$ nm. The
4.5. COOPERATION OF THERMAL ACTIVATION AND CLIMB

Figure 4.12: Strain rate vs. yielding stress curve, showing thermal-activation-dominant region and climb-dominant region under different temperature.

value of thermal parameter takes from Ayas et al. [1], where the temperature $T = 823$ K. The vacancy diffusivity $D_v$ is $2 \times 10^{-13}$ m$^2$s$^{-1}$, the reference concentration $c_0$ is $3 \times 10^{-7}$ µm$^3$, the capture radius $r_c$ is $50b$ and the atomic vacancy volume $\Omega$ is $1.1 \times 10^{-11}$ µm$^3$. The crystallography is represented by two slip systems with angles equal to $\varphi_1 = 30^\circ$ and $\varphi_2 = 150^\circ$, with slip plane spacing $5b$. Sources are randomly distributed with a density of $25$ µm$^{-2}$. Each source is randomly assigned a nucleation strength from a Gaussian distribution with a mean of $\tau_s = 50$ MPa and a standard deviation $\Sigma_s = 0.2\tau_s$. Obstacles are generated on each slip plane from a uniform distribution with a mean of $L_{obs}$, a minimum of $0.5L_{obs}$ and a maximum of $1.5L_{obs}$. We chose $L_{obs} = 0.2$, $0.4$, $0.6$ µm and $\sigma_Y = 300$ MPa. Obstacle strength is calculated from (2.8) for each $L_{obs}$. The mechanical boundary condition is $u_x$ on the right surface $x = -w/2$ is fixed while a uniform stress $\sigma$ is applied on the x direction of the left surface $x = w/2$. The diffusion boundary condition is the bottom surface $y = -h/2$ and the top surface $y = h/2$ maintain constant vacancy concentration $c_0$ and surface $y = -w/2$ and $y = w/2$ are zero flux. Define normalized parameter $\bar{\sigma} = \sigma/\sigma_Y$. We use four different applied stress $\bar{\sigma} = 0.3$, $0.5$, $0.7$ and $0.8$. 

\[ \begin{align*}
\text{700 K} & \quad \begin{array}{c}
\text{By thermal} \\
\text{Transition}
\end{array} \\
\text{800 K} & \quad \begin{array}{c}
\text{By climb} \\
\text{By thermal} \\
\text{Transition}
\end{array} \\
\text{823 K} & \quad \begin{array}{c}
\text{By climb} \\
\text{By thermal}
\end{array}
\end{align*} \]
4.5. COOPERATION OF THERMAL ACTIVATION AND CLIMB

Figure 4.13: Geometry and boundary conditions of the creep problem with two active slip systems, loaded by constant $\sigma$

![Geometry and boundary conditions of the creep problem](image)

Figure 4.14: Creep strain as a function of normalized applied stress $\bar{\sigma}$ under 823 K when dislocation climb is enabled for $L_{\text{obs}}$ (a) 0.2 $\mu$m, (b) 0.4 $\mu$m and (c) 0.6 $\mu$m

![Creep strain as a function of normalized applied stress](image)

Creep strain rate $\dot{\varepsilon}$ as a function of time $t$ with climb only case is show in Fig. 4.14. The cases considering both climb and thermal activation are plotted in Fig. 4.15. Comparing with Fig. 4.14(a) and Fig. 4.15(a), we see that when $\bar{\sigma}$ is small, the climb is dominant. When $\bar{\sigma}$ is large the thermal activation is dominant such that the material cannot resist creep strain. The observation agree with the pileup case in Section 4.5.1. And we can achieve much longer time without scaling the parameter with TADD.
4.6 Summary

We present a new superposition framework for diffusion-assisted climb. First, this framework captures the local climb rate of dislocation in both transient and steady problem. Second, by incorporating a continuous source, this framework operates in a wide range of time scale without increasing the computational complexity. This framework is also able to capture the transient climb rate in a time scale that is comparable to dislocation glide and automatically collapse to steady state solution in the long time. Third, this framework considers the finite body effect in a rigorous way, providing access to solve a more general problem.

Figure 4.15: Creep strain as a function of normalized applied stress $\tilde{\sigma}$ under 823 K when both climb and thermal activation is enabled for $L_{obs}$ (a) 0.2 $\mu$m, (b) 0.4 $\mu$m and (c) 0.6 $\mu$m.
CHAPTER 5

CONCLUSION AND FUTURE WORK

5.1 Conclusion

The plastic behavior at micron scale observed by experiments cannot be predicted by the conventional continuum plasticity model. Therefore, discrete dislocation dynamics methods have been developed over the last two decades as a means to study plastic deformation as collective motion dislocations, rather than a continuum flow. Since the interaction among dislocations and with other material defects is considered, DDD provides fundamental understanding of strengthening/hardening phenomena and of size effects in plasticity. However it is very difficult for DDD to reach experiment-level of strain rate ($\leq 10^{-3}\text{s}^{-1}$) or time scale ($\geq 1\text{s}$) since it keeps tracking the dislocation glide at very small time step ($10^{-11} \sim 10^{-10}\text{s}$). So the kinetics which is sensitive to the dislocation pattern that happens at larger time scales is missing. However, such kinetics as thermal activation or diffusion assisted climb is very important to creep and fracture at high temperature.

Motivated by the need for a general and robust computational framework to extend discrete dislocation plasticity (TADD) to arbitrary time scales, we develop thermal assisted discrete dislocation plasticity model where the glissile time scale is
5.1. CONCLUSION

eliminated by using energy minimization to find equilibrium positions of dislocations. Also, the short range effect occurs at the same order at the glissile time scale is treated as discrete event that alters the energy of the body. Thus, TADD provides access to strain rates and mechanisms of practical interest that were previously inaccessible by DDD simulations. We have proved that TADD agrees with continuum dislocation theory. It shows the similar dislocation pattern evolution with DDD but operates at a wide range of the time scales without increasing the computational cost. This implies that TADD solves the dislocation glide at an arbitrary time scale, which paves the way to incorporate thermal activation or other thermal processes.

Mechanics of a dislocation that is thermally activated over an obstacle field is the first problem we attack. In addition to the traditional parameters required for DDD, we introduce only one extra parameter $\Delta G^*$, the energy barrier for dislocation interaction with obstacles. The nature of this barrier is quite general in our model, and sophisticated atomic-scale data can be used as input to model different alloys. As it stands, the model is most suited to study materials in which the zero temperature response is predominantly controlled by fixed non-shearable obstacles, such as precipitate strengthened alloys (Al-6XXX, Al-Cu and Al-Li). The computational performance of our model across a wide temperature range and strain rates varying over 6 orders of magnitude is comparable to traditional DDD simulations run at a strain rate $\sim 10^2 \text{s}^{-1}$. Our model thus provides a new outlook on modeling strain rate effects at the appropriate temporal scales with discrete dislocations and will be a major advance in examining fracture, fatigue and creep in materials where plastic flow is controlled by obstacles to dislocation motion.

For diffusion assisted climb, we have established a new framework to solve the auxiliary diffusion problem to eliminate the deficiency of the existing model. First, by replacing the dislocation with a continuous source of vacancy, our approach satisfies the time-dependent governing equation and can find compute the rate of climb of
dislocations analytically at arbitrary temporal scales. This solution allows capturing
the dislocation climb accurately where the transient process is dominant such as
interaction with interface, which steady state fails to predict. Our approach also
solves the transient problem at arbitrary time scales. A previous framework [1] which
integrates the instantaneous source numerically operates only at the dislocation glide
time scale (~nanosecond). Second it accounts for coupling of vacancy concentration
fields between dislocations that are close together. This coupling, very important
in high dislocation density or large time scale, is not considered with steady state
framework [65, 77] before and only was solved by recent work of Gu et al. [76]. These
two features make the proposed methodology a universal framework of dislocation
climb.

After incorporating both thermal activation and climb into TADD, we are standing
at a new position to model the plasticity at micron scale that DDD could not
provide. That is modeling the plastic behavior by dislocation pattern evolution at
a time scale comparable to the experiment. TADD enables the addition of more
thermally activation processes while maintaining the information provided by DDD.
It offers the opportunity to examine the individual mechanisms in isolation from the
complicated interactions or superposition that naturally occurs during experiments.
In this context, TADD would provide a quantitative, mechanism-based representa-
tion to the competing thermal processes which is significantly important to creep and
fatigue.

5.2 Future work

In the next step, we would like to extend the dislocation climb framework in Chapter 4
to three dimensional case. Here we propose a possible approach. First the dislocation
loop in 3d is divided into several piece-wise straight segments, depicted in Fig. 5.1(a).
5.2. FUTURE WORK

Figure 5.1: Hierarchical schematic to model dislocation loop as a continuous source:
(a) the dislocation loop operates as several piece-wise straight sources with finite length
(b) a line source with finite length $2H$ and radius $r_c$ can be treated as integral
of spherical point source (c) spherical source with constant concentration within $r_c$.

Each segment is treated as a line source with finite length $2H$. The solution of finite length can be obtained by an integral along the local $z$ axis while each infinitesimal length is regarded as point source, illustrated in Fig. 5.1(b). Each point source is boundary value problem (4.6) with initial and boundary conditions, shown in Fig. 5.1(c),

$$ c(r > r_c, 0) = 0, \quad c(r_c, t) = c^e, \quad c(\infty, t) = 0 \quad (5.1) $$

The solution is

$$ c(r, t) = c^e r_c \frac{r}{r} \text{erfc} \left( \frac{r - r_c}{2\sqrt{D_v t}} \right) \quad (5.2) $$

where $\text{erfc}(z) = 1 - \text{erf}(z)$ and $\text{erf}(z)$ is error function. For a line source with finite length, the solution is [109]

$$ c(r, z, t) = c^e r_c \int_0^H \left\{ \frac{\text{erfc} \left( \frac{\sqrt{(r-r_c)^2+(z-h)^2}}{2\sqrt{D_v t}} \right)}{\sqrt{(r-r_c)^2 + (z-h)^2}} + \frac{\text{erfc} \left( \frac{\sqrt{(r-r_c)^2+(z+h)^2}}{2\sqrt{D_v t}} \right)}{\sqrt{(r-r_c)^2 + (z+h)^2}} \right\} \, dh \equiv c^e S(r, z, t) \quad (5.3) $$
5.2. FUTURE WORK

So for dislocation ensemble with \( n \) segments with the equilibrium concentration on the mid point is \( c_i^{eq} \) \((i = 1..n)\), then

\[
\sum_{j=1}^{n} S(r_{ij}, z_{ij}, t) c_i^* = c_i^{eq} - c^\infty
\]

(5.4)

where \((r_{ij}, z_{ij})\) is the local coordinate of mid point of segment \( i \) in the frame of segment \( j \) with the origin at the mid point of segment \( j \). As we can expect, the evaluation of \( S(r_{ij}, z_{ij}, t) \) in (5.4) is very expensive and there is no close form approximation at hand. However in the case that \( 2H \gg r_c \), the 2d framework given in in Chapter 4 can be directly applied.

In future, we would like to incorporate thermal activation into 3d as well. Just like we do in this work, combine thermal activation with dislocation climb at arbitrary time scale and see what make the plastic behavior differently in 3d. Also adding more physics such as forest hardening would make discrete dislocation plasticity more suitable to practical applications.
REFERENCES


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REFERENCES


APPENDICES

A  Evaluate flux for multiple dislocations

From the superposition of concentration

\[ c(x) = \sum_{i=1}^{n} \tilde{c}_i(x, x_i) + \hat{c}(x) \]  

(A.1)

by applying gradient we have

\[ J(x) = -D_v \nabla c(x) = -D_v \sum_{i=1}^{n} \nabla \tilde{c}_i(x, x_i) - D_v \nabla \hat{c}(x) \]  

(A.2)

Now for a close contour \( \Gamma_i \) around dislocation \( i \), shown in Fig. A.1(a), the flux around dislocation core region is

\[ \oint_{\Gamma_i} n \cdot J \, ds = -D_v \oint_{\Gamma_i} n \cdot \nabla \tilde{c}_i(x, x_i) \, ds \]

\[ - D_v \sum_{j=1, j \neq i}^{n} \oint_{\Gamma_i} n \cdot \nabla \tilde{c}_i(x, x_i) \, ds \]

\[ - D_v \oint_{\Gamma_i} n \cdot \nabla \hat{c}(x) \, ds \]  

(A.3)
A. EVALUATE FLUX FOR MULTIPLE DISLOCATIONS

A.1 Self-contribution to the flux

The first term on the right hand side of (A.1) is directly evaluated. For transient case, by (4.16)
\[ I^\text{self}_i = -2\pi r_c D_v \left[ \frac{\partial c}{\partial r} \right]_{r=r_c} = \frac{2\pi D_v c^*_i}{\ln \left( 1 + \sqrt{\pi t} \right)} \]  \hspace{1cm} (A.4)

For steady state case,
\[ I^\text{st}_i = \frac{2\pi D_v c^*_i}{\ln \left( R^\infty / r_c \right)} \]  \hspace{1cm} (A.5)

A.2 Flux contribution from other dislocations

For the second term, draw a closed contour shown in Fig. A.1(b) and apply divergence theorem
\[ D_v \oint_{\Gamma_1 + \Gamma_r + \Gamma_R + \Gamma_+ + \Gamma_-} \mathbf{n} \cdot \nabla \bar{c}_j (x, x_j) \, ds = \iint_V D_v \nabla \cdot (\nabla \bar{c}_j) \, dv \]  \hspace{1cm} (A.6)

For transient case, since
\[ D_v \oint_{\Gamma_1 + \Gamma_-} \mathbf{n} \cdot \nabla \bar{c}_j (x, x_j) \, ds = 0 \]  \hspace{1cm} (A.7)

and by divergence theorem to Fig.A.1(c)
\[ D_v \oint_{\Gamma_r + \Gamma_R} \mathbf{n} \cdot \nabla \bar{c}_j (x, x_j) \, ds = \iint_{V^+ V^-} D_v \nabla \cdot (\nabla \bar{c}_j) \, dv \]  \hspace{1cm} (A.8)

put (A.7) and (A.8) into (A.6) and after reordering the terms, we have
\[ D_v \oint_{\Gamma_i} \mathbf{n} \cdot \nabla \tilde{c}_j (\mathbf{x}, \mathbf{x}_j) \, ds = - \iiint_{V^-} D_v \nabla \cdot (\nabla \tilde{c}) \, dv \]
\[ = - \iiint_{V^-} D_v \frac{1}{r} \frac{\partial}{\partial t} \left(r \frac{\partial c}{\partial r}\right) \, dv \]  
(A.9)

Substituting the concentration profile (4.15) into (A.9)
\[ D_v \oint_{\Gamma_i} \mathbf{n} \cdot \nabla \tilde{c}_j (\mathbf{x}, \mathbf{x}_j) \, ds = - \frac{4\pi D_v c_j^*}{R_j^2 \ln R_j^2 - R_j^2 + 1} \]  
(A.10)

and putting into the second term of the right hand side of (A.1), we have
\[ I_i^{\text{other}} = \sum_{j=1, j \neq i}^{n} \frac{4\pi D_v c_j^*}{R_j^2 \ln R_j^2 - R_j^2 + 1} \]  
(A.11)

For steady state case, since \( \nabla^2 c = 0 \), the flux is zero.

A.3 Flux contribution from complementary problem

For the third term, draw a closed contour \( \Gamma_i \). It equals to negative value of line integral \( \Gamma_i^- \), shown in Fig. A.2. Apply divergence theorem to \( \Gamma_i^- \)
\[ \oint_{\Gamma_i} \mathbf{n} \cdot \nabla \tilde{c} (\mathbf{x}, \mathbf{x}_i) \, ds = - \oint_{\Gamma_i^-} \mathbf{n} \cdot \nabla \tilde{c} (\mathbf{x}, \mathbf{x}_i) \, ds = - \iiint_{V^-} \nabla \cdot (\nabla \tilde{c}) \, dv \]  
(A.12)

For the transient problem, by substituting the governing equation (4.6) into (A.12), we have
\[ D_v \oint_{\Gamma_i} \mathbf{n} \cdot \nabla \tilde{c} (\mathbf{x}, \mathbf{x}_i) \, ds = - \iiint_{V^-} D_v \nabla \cdot (\nabla \tilde{c}) \, dv = - \iiint_{V^-} \frac{\partial \tilde{c}}{\partial t} \, dv \]
\[ \approx -\pi r_e^2 \frac{\partial \tilde{c}(\mathbf{x}_i)}{\partial t} = -\pi r_e^2 \frac{\partial \tilde{c}(\mathbf{x}_i)}{\partial t} \]  
(A.13)
B. DETERMINE THE TIME STEP FOR DIFFUSION PROBLEM

Then, the flux is

$$I^{\text{back}}_i = \pi r^2 c \frac{\partial \tilde{c}(x_i)}{\partial t}$$  \hspace{1cm} (A.14)

For steady state case, since $\nabla^2 c = 0$, the flux is zero.

**B Determine the time step for diffusion problem**

This part estimates the maximum time step required by the dislocation climb framework by [1]. Since the glide time scale has been eliminated, the time step can be
estimated by diffusivity

\[ \Delta t \equiv \alpha \frac{r_c^2}{D} \]  \hspace{1cm} (B.15)

We would like to chose larger \( \alpha \) to speed up the algorithm meanwhile maintain the convergence. Since the instantaneous source decrease very fast. We take the value of first few step to access the largest suitable \( \alpha \). Here the time step is estimated by single dislocation climb in the infinite media. Assume that dislocation has discrete climb distance. It would not climb until the accumulated climb distance is greater than slip plane spacing. Also we assume constant climb force. Therefore, consider \( \Delta t \equiv \alpha \frac{r_c^2}{D} \) and non-dimensional parameter \( \bar{D} \equiv \frac{D}{Kr_c} \). So, for the first step

\[
\begin{align*}
    c^{(\Delta t)} &= c_0 + \frac{K \Delta t}{2r_c} \left( c_{eq} - c^{(0)} \right) \\
    &= c_0 + \frac{\alpha}{2} \frac{K r_c}{D} \left( c_{eq} - c_0 \right) \\
    &= c_0 + \frac{\alpha}{2} \bar{D} \left( c_{eq} - c_0 \right)
\end{align*}
\]

(B.16)

The constraint is that \( c^{(\Delta t)} \leq c_{eq} \), then \( c_0 + \frac{\alpha}{2\bar{D}} \left( c_{eq} - c_0 \right) \leq c_{eq} \). So we arrive at

\[ \alpha \leq 2\bar{D} \]  \hspace{1cm} (B.17)

In our test case, \( \bar{D} \) takes value of 0.1, 1 and 10. Therefore the maximum value of \( \alpha \) is 0.2. The paper [1] reported \( \alpha = 0.64 \) in single dislocation climb which we disagree. Later they used a \( \Delta t = 0.03 \) ns as time step which is corresponding to \( \alpha = 0.038 \). Here we take \( \alpha = 0.05 \) as a unified time step.