A Multi-Scale Simulation Approach to Deformation Mechanism Prediction in Superalloys

Dissertation

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of The Ohio State University

By

Duchao Lv

Graduate Program in Materials Science and Engineering

The Ohio State University

2016

Dissertation Committee:

Yunzhi Wang, Advisor

Michael Mills

Stephen Niezgoda
Copyright by

Duchao Lv

2016
Abstract

High-temperature alloys in general and superalloys in particular are crucial for manufacturing gas turbines for aircraft and power generators. Among the superalloy family, the Ni-based superalloys are the most frequently used due to their excellent strength-to-weight ratio. Their strength results from their ordered intermetallic phases (precipitates), which are relatively stable at elevated temperatures. The major deformation processes of Ni-based and Co-based superalloys are precipitate shearing and Orowan looping. The key to developing physics-based models of creep and yield strength of aircraft engine components is to understand the two deformation mechanisms mentioned above. Recent discoveries of novel dislocation structures and stacking-fault configurations in deformed superalloys implied that the traditional anti-phase boundary (APB)-type, yield-strength model is unable to explain the shearing mechanisms of the $\gamma''$ phase in 718-type (Ni-based) superalloys. While the onset of plastic deformation is still related to the formation of highly-energetic stacking faults, the physics-based yield strength prediction requires that the novel dislocation structure and the correct intermediate stacking-fault be considered in the mathematical expressions. In order to obtain the dependence of deformation mechanisms on a material’s chemical composition, the relationship between the generalized-stacking-fault (GSF) surface and its chemical composition must be understood. In addition to the stacking-fault energy, particle
morphology and elastic energy control the local activation of strong mechanisms, which leads to the coexistence of multiple deformation modes. For some deformation scenarios in which one precipitate phase and one mechanism are dominant (e.g., Orowan looping), their use in industry requires a fast-acting model that can capture the features of the deformation (e.g., the volume fraction of the sheared matrix) and reduces lost time by not repeating fine-scale simulations.

The objective of this thesis was to develop a multi-scale, physics-based simulation approach that can be used to optimize existing superalloys and to accelerate the design of new alloys. In particular, density functional theory (DFT) was used to calculate the GSF surface of the $\gamma''$ phase in the 718-type superalloy. The atomic structure, fault energy, and stability of several typical stacking faults were determined. In addition, the deformation pathways inside the $\gamma''$ particles were identified, and the dislocation emissions were predicted. Many novel dislocation sources inside the $\gamma''$ particles were simulated by using the phase-field method, which predicts and explains the dislocation configurations that appear during the deformation process or that are left as debris. Moreover, based on the stacking-fault energies in the available literature, we calculated the dependence of the chemical composition of the GSF surface of the $\gamma'$ phase in Co-based, CoNi-based, and Ni-based superalloys. The phase-field simulation, which used the GSF surfaces as inputs, explained the relationship between the shearing mechanism and chemical composition.

By considering the morphology of the particles and the elastic energy within the phase-field simulation, the coexistence of multiple stacking faults was observed in the equilibrium microstructure. Thus, two fast-acting models were developed by using the
modified analytic expressions of particle shearing and Orowan looping. These expressions were calibrated by using the GSF surface and the simulation of the phase-field, and they were used to predict the yield strength of 718-type superalloy and the localized creep features of the $\gamma/\gamma'$ microstructure. The fast-acting yield models were trained by the available experimental results. Since the chemical re-ordering and the segregation effects are not considered in this work, the fast-acting models are designed to predict mechanical behaviors at the room temperature and the intermediate temperature.
Dedication

This document is dedicated to Prof. Leaf Huang, my grandfather Hongyi Du, and my wife Yongyu Yan.
Acknowledgments

I am fortunate to have studied in the research group of my advisor, Dr. Yunzhi Wang. He has been guiding me on my academic journey ever since 2011. I have benefitted a lot from the invaluable environment that he has created for this students. I want to give my sincere thanks and respects to Dr. Michael Mills and Dr. Stephen Niezgoda, for the valuable encouragements and insightful suggestions that they have offered me during my graduate study.

I want to thankfully acknowledge the financial support of this research through the Materials Affordability Initiative Program on Integrated Microstructure and Process Modeling of Alloy 718 Aerospace Components. I also want to acknowledge the support of the NSF DMREF program under grant # 1534826.

My deep appreciation must also be given to those who have supported and accompanied me in the past five years, including Prof. Maryam Ghazisaeidi, Prof. Wolfgang Windl, Prof. Suliman Dregia, Prof. Ju Li, Prof. Tresa Pollock, Donald, McAllister, Timophy Smith, Ning Zhou, Pengyang Zhao, Rongpei Shi, Yipeng Gao, Xiaojin Ke, Liang Qi and Michael Titus. Many thanks go to my friends including Barry Yang, Lingfeng Zhang, Dennis Ong, Timmy Ong, Quanlin Guo, James Tsai, Deborah Lin, Joshua Zhang, Xiaoli

I also want to give my thanks to my parents Fangfang Du and Haifeng Lv, and my wife Yongyu Yan.
Vita

2008.........................................................B.S., Electrical and Computer Engineering, Xi’an Jiao Tong University, China

2011..........................................................M.S. Electrical and Computer Engineering, Xi’an Jiao Tong University, China

2014..........................................................M.S. Materials Science and Engineering, The Ohio State University, Columbus, Ohio

2014 to present .........................................Graduate Research Assistant, Materials Science and Engineering, The Ohio State University, Columbus, Ohio

Publications


Fields of Study

Major Field: Materials Science and Engineering
# Table of Contents

Abstract ........................................................................................................................................ ii

Dedication ..................................................................................................................................... v

Acknowledgments ...................................................................................................................... vi

Vita ............................................................................................................................................... viii

List of Tables .............................................................................................................................. xiii

List of Figures ............................................................................................................................. xv

Chapter 1: Introduction .............................................................................................................. 1

1.1. The industrial applications of superalloys ................................................................. 1

1.2. Precipitate size distribution and volume fraction ......................................................... 2

1.3. Morphology and elastic energy of the precipitate ......................................................... 3

1.4. Stacking fault of precipitate ............................................................................................ 5

1.5. Orowan looping of precipitate ......................................................................................... 12

1.6. Transition from shearing to looping ............................................................................. 15

1.7. Dislocation configurations in superalloys ..................................................................... 18

1.8. Generalize-stacking-fault (GSF) potential surface ...................................................... 21
Chapter 2: Generalized-Stacking-Fault (GSF) Potential Surfaces of Precipitate Phases

2.1. Fundamental properties of γ'' phase from DFT calculation
2.2. Stacking faults in γ'' phase
2.3. GSF energy surface of γ'' phase from DFT calculation
2.4. Stability of stacking faults
2.5. GSF surface of γ phase (L1_2 structure)
2.6. Summary

Chapter 3: Deformation Mechanisms of 718-type Superalloys

3.1. Phase-field simulation of dislocation shearing of γ'' precipitates
3.2. Dislocation core structure in the deformation process related to AC+AB
3.3. Deformation of 718-type microstructure
3.4. Dominating deformation mechanism
3.5. Misfit strengthening
3.6. Composite particle formation: an aspect of the elastic energy
3.7. Discussion
3.8. Summary

Chapter 4: Deformation Mechanisms of the γ/γ' Microstructure in Superalloys
| Chapter 4: Deformation of Spherical Particles | 4.1. Deformation of spherical particles | 136 |
| Chapter 4: Formations of SISF Island | 4.2. Formation of SISF island | 152 |
| Chapter 4: Stability of the SISF Island | 4.3. Stability of the SISF island | 160 |
| Chapter 4: Summary | 4.4. Summary | 163 |
| Chapter 5: Fast-Acting Models of Superalloy Deformation | 5.1. Fast-acting Orowan looping model | 165 |
| Chapter 5: Dislocation Activation Diagram (DAD) of Local Channel Width | 5.2. Dislocation activation diagram (DAD) of local channel width | 168 |
| Chapter 5: Local Channel Map | 5.3. Local channel map | 173 |
| Chapter 5: Orowan Looping Simulation at 80Ksi/1300°F | 5.4. Orowan looping simulation at 80Ksi/1300°F | 178 |
| Chapter 5: Fast-Acting Yield Strength Model of 718-Type Superalloy | 5.5. Fast-acting yield strength model of 718-type superalloy | 180 |
| Chapter 5: Summary | 5.6. Summary | 200 |
| Chapter 6: Summary and Future Work | 6.1. Summary | 203 |
| Chapter 6: Future Work | 6.2. Future Work | 205 |
| Bibliography | Bibliography | 209 |
List of Tables

Table 1. The lattice parameters and elastic modulus (GPa) of $\gamma^\prime$ phase. ...................... 37
Table 2. The displacement vector and stacking fault energies. ........................................... 40
Table 3. The parameters of the GSF surfaces of the $\gamma'$ phases. ..................................... 49
Table 4. The parameters of the GSF surfaces of the $\gamma$ matrix...................................... 50
Table 5. Some physical parameters used in this chapter. .................................................. 136
Table 6. The temperature-independent model parameters.................................................. 183
Table 7. The model parameters related to shear modulus (temperature-dependent). [91] .......... ................................................................. 183
Table 8. The model parameters related to stacking-fault energy (temperature-dependent). .......... ................................................................. 183
Table 9. The model parameters related to lattice stress (solid solution hardening + forest dislocation hardening, temperature-dependent). [27] ........................................ 184
Table 10. The comparison of average channel width between $\gamma^\prime$ particles determined from the precipitate microstructures generated by the phase field simulations and calculated from the analytic expression.................................................. 187
Table 11: The stacking fault ribbon and the related Burgers vector for each variant of $\gamma''$ ................................................................. 189
Table 12. The $\gamma''$ phase strengthening mechanisms list .............................................................. 193

Table 13: The deformation mechanisms in the $\gamma''$ particles when a AC+AB ( $\frac{1}{2} <112>$) dislocation is considered ........................................................................................................... 195
List of Figures

Figure 1. Alloys in an aerospace engine. The red color indicates the nickel-based superalloys. ................................................................. 1

Figure 2. The temperature dependences of the (111)-type and the (100)-type APB energies in the γ’ phase (L1$_2$, Ni$_3$Al) of the Ni-based superalloy. This is a theoretic result which is based on a thermodynamic database and the calculated by D. M. Collins et al. [22]. ................................................................. 8

Figure 3: The temperature dependences of the stacking-fault energy in the L1$_2$ phase. This is a theoretic result which is based on the mean-field approach by A.G. Khachaturyan [23]. ................................................................................. 10

Figure 4. The temperature dependences of the APB energy in the γ’ phase (L1$_2$, Ni$_3$(Al, Hf)). This is an experimental result [25]. When temperature > 600K, there is a fast-dropping of the APB energy. ................................................................................. 11

Figure 5: The spatial arrangement of ellipse particles which is applied in the inter-particle distance calculation by M.R. Ahmadi [26]. A periodic triangular array is assumed. ...... 12

Figure 6. The temperature dependence of the lattice friction (SSH + dislocation forest) according to experimental measurements [27]. Several Ni-based alloys are investigated and the results for the Ni-13.1Cr are applied in the yield strength model in Chapter 5. .. 15
Figure 7. The particle-size-distribution dependence of the yield strength according to the theoretic calculations [28]. The average particle size increases with the aging time. ...

Figure 8. The shearing mechanism of the $\gamma'$ particle by an $<112>$-type dislocation group [10]. The deformation process firstly creates SISF area which is later consumed by the following APB and SESF. The final debris of this deformation process is an SESF whose formation requires the chemical re-ordering.

Figure 9. TEM picture of an (111) cross section sheared by the $<112>$ type dislocation group in the TMS-82+ superalloy. Both intrinsic (SISF) and extrinsic (SESF) faults are observed. [18]

Figure 10. A phase-field simulation revealed the dislocation core structure of the $<112>$ type dislocation group which has already interacted with a $\gamma'$ particle. Chemical re-ordering was not considered in this simulation. The SISF, APB, and CSF appear as the intermediate stacking ribbons of the deformation process. [18]

Figure 11. A GSF surface of the $\gamma'$ phase (L1$_2$, Ni$_3$Al) was calculated by fitting an analytic expression with the DFT calculations. [20]

Figure 12. A TEM picture and a conceptual diagram which give one possible explanation of the dislocation configuration in the $\gamma''$ dominating superalloy (e.g., 718-type) [2].

Figure 13. The 3-D diagrams of the crystalline structures of the $\gamma$ (FCC, Ni), $\gamma'$ (L1$_2$, Ni$_3$Al) and $\gamma''$ (D0$_{22}$, Ni$_3$Nb) phases.

Figure 14. The six-layer supercells of a DO$_{22}$ structure containing various stacking faults.
Figure 15. The atomistic configurations viewed along the [111] of a D0\textsubscript{22} structure showing the APB, CSF, SISF, APB-like stacking fault, and CSF-like stacking fault. The black and blue dashed lines indicate the mirror planes.

Figure 16. The generalized-stacking-fault (GSF) potential energy surface of the equivalent 111\textgamma plane in \gamma'' phase. The red-dashed box indicates the periodically repeating unit of the GSF-surface. The Burgers vectors of different faults (indicated by the arrows) are given in the legend. The blue arrow indicates the displacement along ½ [11-2]. The white arrow indicates the displacement along ½ [-110]. The yellow arrow indicates the displacement along 1/6[-211]. The green arrow indicates the displacement along 1/6[-12-1].

Figure 17. GSF energy landscapes along special deformation pathways: (a) along ½ [11-2]; (b) along [-110]; (c) along 1/6 [-211] (blue solid line) and 1/6 [-12-1] (red dashed line); (d) along 1/6 [-12-1] (blue solid line) and 1/6 [-211] (red dashed line).

Figure 18. The composition dependence of the stacking fault energies. The data points are obtained for the Ni-based, Co-based and CoNi-based superalloys.

Figure 19. The composition dependence of GSF surface. The GSF surfaces are obtained by fitting an analytic expression with data points which are obtained for the Ni-based, Co-based and CoNi-based superalloys. The 3-fold rotational symmetry is revealed by the white triangular, and the mirror planes are plotted with the white dashed lines.

Figure 20. The GSF potential energy surfaces for the three \gamma'' variants obtained from DFT calculation. Symbols which represent stacking faults are explained in the legend, and the corresponding Burgers vectors of the faults are shown in the inset.
Figure 21. The crystalline (stacking fault) energy contour displays the interaction between an AB dislocation and the three variants of γ″ particles. The top figures indicate the total energy contour and the bottom figures show schematically the corresponding dislocation and fault configurations in both γ″ and γ' phases. The white arrow indicates the Burgers vector (AB) of the full dislocation and the red arrow indicates the applied stress direction.

Figure 22. (Frame 1 and Frame 2) The crystalline (stacking fault) energy contour displays the interaction between AC+AB dislocation pair and of γ″ particles (grey color). Figures in the first row indicate the total energy contour, and the figures in the remaining rows show dislocation/SF configurations at three successive instances. The white arrows indicate AB and AC Burgers vectors, and the red arrow displays the applied stress direction.

Figure 23. (Frame 3 and Frame 4) The crystalline (stacking fault) energy contour displays the interaction between AC+AB dislocation pair and of γ″ particles (grey color). Figures in the first row indicate the total energy contour, and the figures in the remaining rows show dislocation/SF configurations at three successive instances. The white arrows indicate AB and AC Burgers vectors, and the red arrow displays the applied stress direction.

Figure 24. The AC+AB dislocation core profile inside the Variant 1 of the γ″ particles (Frame 1). The ISF and SISF are displayed as the intermediate stacking fault ribbons..
Figure 25. The AC+AB dislocation core profile inside the Variant 1 of the $\gamma''$ particles (Frame 2). The ISF and SISF are displayed as the intermediate stacking fault ribbons. The APB-like stacking fault appears and will transform into an ISF in the next Frame. 63

Figure 26. The AC+AB dislocation core profile inside the Variant 2 of the $\gamma''$ particles (Frame 1). The ISF and SISF are displayed as the intermediate stacking fault ribbons. The APB-like stacking fault appears and will transform into an ISF later. 65

Figure 27. The AC+AB dislocation core profile inside the Variant 2 of the $\gamma''$ particles (Frame 2). The ISF and SISF are displayed as the intermediate stacking fault ribbons. The APB-like stacking fault appears and will transform into an ISF in the next Frame. 66

Figure 28. The AC+AB dislocation core profile inside the Variant 2 of the $\gamma''$ particles (Frame 3). The ISF is the final debris inside the particle. 67

Figure 29. The AC+AB dislocation core profile inside the Variant 3 of the $\gamma''$ particles (Frame 1). The APB-like stacking fault will transform into an ISF in the next Frame. 68

Figure 30. The AC+AB dislocation core profile inside the Variant 3 of the $\gamma''$ particles (Frame 2). The ISF is the intermediate ribbon during the shearing process. 69

Figure 31. The thermodynamic prediction of the dynamic evolution of the volume fraction in the 718-type superalloy. 73

Figure 32 The thermodynamic prediction of the dynamic evolution of the particle size in the 718-type superalloy. 73
Figure 33. The phase-field simulation of the microstructural evolution. Random particle nuclei are initiated in the Frame 1. The growth and the coarsening happen in the Frames 2, 3 and 4.................................................................................................................. 74

Figure 34. The channel map and the particle spatial distribution in the 718-type microstructure. The γ″ particles are displayed in the red color. The cyan-blue lines indicate the channels. The γ′ particles are assumed to be sheared................................. 76

Figure 35. The normalized histogram of the channel width distribution in the 718-type microstructure. ................................................................. 77

Figure 36. The CRSS map of the local Orowan looping strengthening in the 718-type microstructure. The γ″ particles are displayed as the white objects. The value in each triangular patch represents the Orowan looping strengthening to any dislocation loop originated inside the triangular patch. The strengthening (CRSS) is calculated by using the average channel width of triangular patches........................................ 78

Figure 37. The channel width distribution when both the γ′ and γ″ particles are assumed to be looped.................................................................................................................. 78

Figure 38. The normalized histogram of the channel widths distribution in the 718-type microstructure is displayed when both the γ′ and γ″ particles are assumed to be looped. 79

Figure 39. The CRSS map of the local Orowan looping strengthening in the 718-type microstructure. Both the γ″ and γ′ particles are assumed to be looped. The value in each triangular patch represents the Orowan looping strengthening to any dislocation loop originated inside the triangular patch. The strengthening (CRSS) is calculated by using the average channel width of the triangular patch. .......................................................... 79
Figure 40. The phase-field simulation of the interaction between the δC emitted dislocation with the γ' particle. The pinning effect is represented by the creation of the CSF inside the γ' phase. The entire crystal has already been sheared by the BA full dislocation. The GSF energy of the γ' phase is not scaled. .................................................. 81

Figure 41. The phase-field simulation of the interaction between the δC emitted dislocation and the γ' particle. The pinning effect is represented by the Orowan looping around the γ' particle. The entire crystal has already been sheared by the BA full dislocation. The GSF energy of the γ' phase is scaled by a factor of 2. ......................... 82

Figure 42. The phase-field simulation of the interaction between the δC emitted dislocation and the γ'' particle. The pinning effect is represented by the Orowan looping around the γ'' particle. The entire crystal has already been sheared by the AC+AB dislocation group................................................................. 83

Figure 43. The phase-field simulation of the δC+δB emitted dislocation group which is immobile inside the γ matrix. The pinning effect is due to the prohibited dislocation reaction. The entire crystal has already been sheared by the AC+AB dislocation group. 85

Figure 44. The early four frames of the phase-field simulation of the δC+δB emitted dislocation group which moves through the γ'' particle under the applied stress along the δB direction. The Aδ loop is emitted when the δC+δB dislocation group cuts though the Variant 1 particle of the γ'' phase. The Aδ loop is later pinned by the Variant 2 particle of the γ'' phase. The entire crystal has already been sheared by the AC+AB dislocation group. ................................................................. 86
Figure 45. The last four frames of the phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which moves through the $\gamma''$ particle under the applied stress along the $\delta B$ direction. The $A\delta$ loop is pinned by the Variant 2 particle of the $\gamma''$ phase. The only stacking fault debris is the ISF in the Variant 2 particle of the $\gamma''$ phase. The entire crystal has already been sheared by the $AC+AB$ dislocation group. .................................................. 87

Figure 46. The early four frames of the phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which moves through the $\gamma''$ particle under the applied stress along the $\delta C$ direction. The $A\delta$ loop is emitted when the $\delta C+\delta B$ dislocation group cuts through the Variant 2 particle of the $\gamma''$ phase. The $A\delta$ loop is later pinned by the Variant 1 particle of the $\gamma''$ phase. The entire crystal has already been sheared by the $AC+AB$ dislocation group. .................................................................................. 88

Figure 47. The last two frames of the phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which moves through the $\gamma''$ particle under the applied stress along the $\delta C$ direction. The $A\delta$ loop is pinned by the Variant particle of the $\gamma''$ phase. The only stacking fault debris is the ISF in the Variant 1 particle of the $\gamma''$ phase. The entire crystal has already been sheared by the $AC+AB$ dislocation group. .................................................. 89

Figure 48. The early four frames of the phase-field simulation of the $AB$ pair cutting through the Variant 1 particle of the $\gamma''$ phase. The $A\delta+C\delta$ dislocation group is created which is impossible to move since the $A\delta$ and $C\delta$ cannot interact................................................. 90
Figure 49. The last two frames of the phase-field simulation of the AB pair cutting through the Variant 1 particle of the $\gamma''$ phase. The A$\delta$+C$\delta$ dislocation group is created which is impossible to move since the A$\delta$ and C$\delta$ cannot interact. 91

Figure 50. The early four frames of the phase-field simulation of the AB pair cutting through the Variant 3 particle of the $\gamma''$ phase. The $\delta$B+$\delta$C dislocation group is created which is impossible to move since the $\delta$B and $\delta$C cannot interact. 93

Figure 51. The last four frames of the phase-field simulation of the AB pair cutting through the Variant 3 particle of the $\gamma''$ phase. The $\delta$B+$\delta$C dislocation group is created which is impossible to move since the $\delta$B and $\delta$C cannot interact. 94

Figure 52. A deformation process is simulated by the phase-field method when an AC single dislocation interacts with a 718-type microstructure. The AC dislocation is unable to percolate through the microstructure, due to the strong pinning effect from the $\gamma''$ phase. 96

Figure 53. The early stages of a deformation process are simulated by the phase-field method when an AC pair interacts with a 718-type microstructure. The dislocation loops are left at the $\gamma/\gamma''$ boundaries while the $\gamma'$ particles are sheared. 97

Figure 54. The later stages of a deformation process are simulated by the phase-field method when an AC pair interacts with the 718-type microstructure. The dislocation loops are left at the $\gamma/\gamma''$ boundaries while the $\gamma'$ particles are sheared. The leading and trailing ACs are decoupled, which implies a slower deformation rate of the trailing AC. 99

Figure 55. The early stages of a deformation process are simulated by the phase-field method when an AC quadruplet interacts with a 718-type microstructure. The
components of this quadruplet are decoupled, which implies a slower deformation rate.

Figure 56. The later stages of a deformation process are simulated by the phase-field method when an AC quadruplet interacts with a 718-type microstructure. The components of this quadruplet are decoupled, which implies a slower deformation rate. The trailing two ACs are stopped in the vicinity of their initial location.

Figure 57. A deformation process is simulated by the phase-field method when an AC+AB group interacts with a 718-type microstructure. The components of this group are strongly coupled, which implies a relatively high deformation rate. Only the $\frac{1}{2}<116>$ type dislocation loops are left at the $\gamma/\gamma''$ boundaries as the debris. The $\gamma'$ particles are sheared and an APB area is created.

Figure 58. The stacking fault configuration distribution in the Variant 1 of the $\gamma''$ phase. The original structure is dominating, which implies that the Orowan looping happens on the $\gamma/\gamma''$ boundaries of the Variant 1.

Figure 59. The stacking fault configuration distribution in the Variant 2 of the $\gamma''$ phase. The ISF is dominating, which implies that the stacking fault transformation happens in most Variant 2 $\gamma''$ particles. Meanwhile, the restored structure corresponds to the stacking fault transformation from the CSF to the perfect stacking sequence. Very little APB area is observed, which means the traditional AC pair shearing models, which predicts a large amount of APB, indeed fail.

Figure 60. The stacking fault configuration distribution in the Variant 3 of the $\gamma''$ phase. The restored structure is dominating, which implies the stacking fault transformation...
from the CSF to the perfect stacking sequence. Again, very little APB area is observed, which means the traditional AC pair shearing models indeed fail. ................................107

Figure 61. Stacking fault configuration distribution in the $\gamma'$ particles. The restored structure is dominating, which is consistent with the Burgers vector of AC pair. ........108

Figure 62. The stacking fault configuration distribution in the $\gamma$ matrix. The restored structure is dominating, which is consistent with the Burgers vector of the AC pair.....108

Figure 63. The stacking fault configuration distribution in the Variant 1 of the $\gamma''$ phase. The original structure is dominating, which implies that the Orowan looping happens on the $\gamma/\gamma''$ boundaries of the Variant 1.................................................................109

Figure 64. The stacking fault configuration distribution in the Variant 2 of $\gamma''$ phase. The ISF is dominating, which implies that stacking fault transformation happens in most Variant 2 of the $\gamma''$ particles. Meanwhile, the restored structure corresponds to the stacking fault transformation from the CSF to the perfect stacking sequence. Very little area of the restored structure is observed, which means the traditional AC quadruplet shearing models, which predicts a large amount of the restored structure, indeed fail. 110

Figure 65. The stacking fault configuration distribution in the Variant 3 of the $\gamma''$ phase. The restored structure is dominating, which implies the stacking fault transformation from the CSF to the perfect stacking sequence. Again, very little area of the restored structure is observed, which means the traditional AC quadruplet shearing models indeed fail. .................................................................110
Figure 66. The stacking fault configuration distribution in the $\gamma'$ particles. The restored structure is dominating, which is consistent with the Burgers vector of the AC quadruplet.

Figure 67. The stacking fault configuration distribution in the $\gamma$ matrix. The restored structure is dominating, which is consistent with the Burgers vector of the AC quadruplet.

Figure 68. The stacking fault configuration distribution in the Variant 1 of the $\gamma''$ phase. The ISF is dominating, which implies the stacking fault transformation from the APB-like stacking fault to the ISF.

Figure 69. The stacking fault configuration distribution in the Variant 2 of the $\gamma''$ phase. Again, the ISF is dominating, which implies the stacking fault transformation from the APB-like stacking fault to the ISF.

Figure 70. The stacking fault configuration distribution in the Variant 3 of the $\gamma''$ phase. The restored structure is expected to be created the Burgers vector of the AC+AB.

Figure 71. The stacking fault configuration distribution in the $\gamma'$ particles. The APB is dominating, which is consistent with the Burgers vector of the AC+AB.

Figure 72. The stacking fault configuration distribution in the $\gamma$ matrix. The restored structure is dominating, which is consistent with the Burgers vector of the AC+AB.

Figure 73. The interaction between the Variant 1 of the $\gamma''$ phase and the dislocations. The interaction energy density is plotted and represents a repulsive force.

Figure 74. The interaction between the Variant 2 of the $\gamma''$ phase and the dislocations. The interaction energy density is plotted and represents a repulsive force.
Figure 75. The interaction between the Variant 3 of the γ” phase and dislocations. The interaction energy density is plotted and represents a repulsive force.

Figure 76. The interaction between the Variant 1 of the γ” phase and dislocations. The interaction energy density is plotted and represents an attractive force.

Figure 77. The interaction between the Variant 2 of the γ” phase and the dislocations. The interaction energy density is plotted and represents an attractive force.

Figure 78. The interaction between the Variant 3 of the γ” phase and the dislocations. The interaction energy density is plotted and represents an attractive force.

Figure 79. The electron microscopy observation of the composite particles: (a) the cubic-like composite particle[76] ; (b) the hamburger-like composite particle[86]. Generally, the cubic-like particle is of 0.1 um in size, while the length scale of the hamburger-like particle is finer, which is ~10nm.

Figure 80. The stress field of the hamburger-like composite particle, as a function of the volume fraction of the γ’ phase and the space coordination. We adjust the b/a ratio from 0 to 1, indicating from γ” to γ’ particle, while the intermediate state is a hamburger-like composite particle. Here it is the case for the γ” variant 1.

Figure 81. The total elastic energy is calculated as a function of the b/a ratio. There are two lines in this figure. The red line corresponds to a direct mixture of the γ’ and γ” phases under the given volume fractions, where the elastic interaction is neglected. On the black line, the elastic interaction between the γ’ and γ” is considered.

Figure 82. The stress field of the “improper” hamburger-like composite particle, as a function of the volume fraction of the γ’ phase and the space coordination. We adjust the
b/a ratio from 0 to 1, indicating from $\gamma''$ to $\gamma'$ particle, while the intermediate state is a hamburger-like composite particle. Here it is the case for the $\gamma''$ variant 1. .................. 126

Figure 83. The total elastic energy is calculated as a function of the b/a ratio. There are two lines in this figure. The red line corresponds to a direct mixture of the $\gamma'$ and $\gamma''$ phases under the given volume fractions, where the elastic interaction is neglected. On the blue line, the elastic interaction between the $\gamma'$ and $\gamma''$ is considered....................... 128

Figure 84. A TEM picture of the cubic-like $\gamma'$ particles of a Co-based superalloy. ...... 132

Figure 85. A TEM picture of the APB and SISF configurations in the Co-based superalloys [21]........................................................................................................... 133

Figure 86. A deformation process is simulated by the phase-field approach when an AB single dislocation interacts with a $\gamma'$ particle in a Ni-based superalloy. The Orowan looping happens which is due to the high APB energy. ........................................... 137

Figure 87. The early stages of a deformation process are simulated by the phase-field approach when an AB single dislocation interacts with a $\gamma'$ particle in a CoNi-based superalloy. The APB shearing happens which is a result of the relatively low APB energy............................................................... 137

Figure 88. The later stages of a deformation process are simulated by the phase-field approach when an AB single dislocation interacts with a $\gamma'$ particle in a CoNi-based superalloy. The debris structure is APB due to the relatively low APB energy............ 138

Figure 89. A deformation process is simulated by the phase-field approach when an AB single dislocation interacts with a $\gamma'$ particle in a Co-based superalloy. The Orowan looping happens which is due to the high APB energy................................. 138
Figure 90. A 3-D plot [21] shows how an AB dislocation interacts with a cubic-like γ’ particle on (111) plane. The (111) cross section is triangular. The APB area is displayed in yellow color. The blue color indicates the area which has not been sheared. 141

Figure 91. The GSF surfaces of the γ’ phases shows the deformation pathway of the AB+AC dislocation shearing. 142

Figure 92. The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a γ’ particle in a CoNi-based superalloy. The APB shearing happens which is a result of the relatively low APB energy. 143

Figure 93. The Frame 4 of the above simulation is enlarged in order to display the detailed dislocation and the stacking fault configurations. 144

Figure 94. The later stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a γ’ particle in a CoNi-based superalloy. The APB is created as the debris due the relatively low APB energy. 144

Figure 95. The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a γ’ particle in a Co-based superalloy. The SISF shearing happens while a APB area is absent, which is a result of the relatively high APB energy. 145

Figure 96. The Frame 3 of the above simulation is enlarged in order to display the detailed dislocation and the stacking fault configurations. 145

Figure 97. The later stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a γ’ particle in a Co-based superalloy.
The APB is created as the debris while the Aδ dislocation loop is left at γ/γ′ boundary, due the relatively high APB energy. ......................................................... 146

Figure 98. A 3-D plot [21] shows how an AB+AC group interacts with a cubic-like γ′ particle on the (111) cross section. The APB area is displayed in the yellow color. The blue color indicates the area which has not been sheared........................................ 150

Figure 99. A 3-D plot [21] shows how an AB+AC group interacts with a cubic-like γ′ particle on the (111) cross section. The SISF area is displayed in the green color. The blue color indicates the area which has not been sheared................................. 151

Figure 100. A 3-D plot shows two types of the (111) cross sections of a cubic-like γ′ particle............................................................................................................. 152

Figure 101. A triangular (111) cross section of the γ′ phase evolutes, which is simulated by the phase-field approach. ............................................................................. 153

Figure 102. A hexagonal (111) cross section of the γ′ phase evolutes, which is simulated by the phase-field approach. ............................................................................. 154

Figure 103. The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a γ′ particle in a Co-based superalloy. The cross section is triangular. The AB dislocation has already cut through the particle. The APB and SISF are observed to coexist during the deformation. ............................. 156

Figure 104. The final stage of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a γ′ particle in a Co-based superalloy. The cross section is triangular. The APB and SISF coexist in a stable configuration. ........ 156

xxx
Figure 105. The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a $\gamma'$ particle in a Co-based superalloy. The cross section is hexagonal. The AB dislocation has already cut through the particle. The APB and SISF are observed to coexist during the deformation. ........................................ 157

Figure 106. The final stage of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a $\gamma'$ particle in a Co-based superalloy. The cross section is hexagonal. Only the SISF exists in the stable configuration. ............... 157

Figure 107. The stabilized shapes of the $\Lambda\delta$ dislocation loop in the presence and absence of Poisson’s ratio.......................................................... 159

Figure 108. In the Ni-based superalloy, a deformation process is simulated by the phase-field approach when an initial dislocation configuration of the SISF+APB is applied. This initial configuration is stable in the Co-based superalloy. The APB area finally disappears due to the relatively high APB energy. ........................................................................ 162

Figure 109. In the CoNi-based superalloy, a deformation process is simulated by the phase-field approach when an initial dislocation configuration of the SISF+APB is applied. This initial configuration is stable in the Co-based superalloy. The APB area gradually expands and will finally consume all the SISF area, which is a result of the relatively low APB energy.......................................................... 162

Figure 110. A digitalized SEM picture of the HL11 microstructure. The red color indicates the $\gamma'$ particles, and the blue color means the $\gamma$ matrix. ........................................ 169
Figure 111. A DAD diagram is calculated when the average channel width (116 nm) of the above HL11 microstructure is used. The calculation shows that a full dislocation is active.

Figure 112. A deformation process is simulated by the phase-field approach when an AB dislocation interacts with the HL11 microstructure. The area of the ISF activation is obviously larger than the area of the full dislocation percolation.

Figure 113. The later stage of a deformation process is simulated by the phase-field approach when an AB dislocation interacts with the HL11 microstructure. The area of the ISF activation is obviously larger than the area of the full dislocation percolation. The δB dislocation is decoupled from the Aδ dislocation.

Figure 114. The critical channel width, which separates the full dislocation activation and the de-correlation, is characterized by the phase-field simulation.

Figure 115. A DAD diagram is calculated when the critical channel width (67.5 nm) is used. The boundary between the full dislocation activation and the de-correlation lays on the applied stress condition. The applied stress condition is represented by the green dot which is marked by a red dashed circle.

Figure 116. A digitalized ME3 microstructure. The black color indicates the γ' particles, and the white color means the γ matrix. The zone where the following calculations are performed is inside the red dashed box.

Figure 117. The local channels are displayed in the digitalized ME3 microstructure.

Figure 118. A DAD diagram is calculated when the average channel width of the ME3 is used.
Figure 119. A DAD diagram is calculated when the critical channel width of the full dislocation activation is used. The temperature is 1300°F......................................................... 175

Figure 120. A DAD diagram is calculated when the critical channel width of the de-correlation is used. The temperature is 1300°F................................................................. 175

Figure 121. Narrow local channels are displayed in the digitalized ME3 microstructure. The red channels are narrower than the critical channel width of the full dislocation. The blue channels are narrower than the critical channel width of the de-correlation. The loading condition is 80Ksi/1300°F. ............................................................... 176

Figure 122. Narrow local channels are displayed in the digitalized ME3 microstructure. The red channels are narrower than the critical channel width of the full dislocation. The blue channels are narrower than the critical channel width of the de-correlation. The loading condition is 80Ksi/1600°F. Three percolation pathways are indicated by the orange arrows................................................................. 177

Figure 123. Narrow local channels are displayed in the digitalized ME3 microstructure. The blue channels are narrower than the critical channel width. The loading condition is 60Ksi/1300°F. ............................................................... 178

Figure 124. Narrow local channels are displayed in the digitalized ME3 microstructure. The blue channels are narrower than the critical channel width. The loading condition is 60Ksi/1600°F. ............................................................... 178

Figure 125. The percolation simulation is performed when full dislocation is initiated at the simulation box boundaries of (A) the left side, (B) the right side, (C) the lower side, and (D) the upper side. The yellow color means that the matrix has been sheared by the
full dislocation, the cyan blue indicates the de-correlation area, and the dark blue means the inactivation. The \( \gamma' \) particles are displayed in the red color. The percolation distance of the full dislocation is indicated by the black arrow.

Figure 126. The de-correlation and inactivation volume fractions are calculated as the functions of the tertiary volume fraction and the service temperature.

Figure 127: The flowchart of the model development.

Figure 128: The particle size distribution obtained from the phase-field simulations.

Figure 129: The typical examples of a unimodal log-normal particle size distribution when the cut-off particle size is chosen to be 80 nm.

Figure 130: The channel widths among the \( \gamma'' \) particles (the blue lines in (b)) identified for the precipitate microstructure shown in (a) generated by the phase field simulations.

Figure 131. The overall framework of the fast-acting yield strength model.

Figure 132. The meanings of the mechanism population and the critical particle size in a given particle size distribution.

Figure 133. The structure of the fast-acting yield strength model.

Figure 134: The comparison between the model prediction and the experimental measurement of the yield strength of IN718 as a function of the temperature.

Figure 135: The critical particle size as a function of the average particle size and the service temperature.

Figure 136: The population of each deformation mechanism as a function of the average particle size and the service temperature.
Figure 137: The strength of each deformation mechanism as a function of the average particle size and the service temperature. ................................................................. 199

Figure 138: The total yield strength as a function of the average particle size. .......... 199

Figure 139: The prediction of the yield strength as a function of the total volume fraction of the precipitates, and the average particle size at the room temperature. A log-normal particle size distribution is used in this calculation. .................................................. 200

Figure 140: A framework of the statistical analysis of the representative microstructure. .......................................................................................................................... 208
Chapter 1: Introduction

1.1. The industrial applications of superalloys

Superalloys are crucial for manufacturing gas turbines, which are the key components of aerospace and power generators. Superalloys are used extensively in extreme service conditions, such as high loading stress and high temperature. They exhibit an extraordinary combination of creep resistance, fatigue resistance, oxidation resistance, and mechanical strength. Ni-based superalloy, which has an excellent strength-to-weight ratio, is the most frequently used member of the superalloy family. For decades, many efforts have been made to understand the underlying deformation mechanisms that contribute to superalloys’ high strength-to-weight ratio.

Figure 1. Alloys in an aerospace engine. The red color indicates the nickel-based superalloys.
In turbine engines, superalloys are used extensively for hot section disks and airfoils. Many other industrial applications also take advantage of superalloys’ superior properties, for example, they are used as components in nuclear power systems, metal processing, chemical and petrochemical systems, and medical devices [1].

1.2. **Precipitate size distribution and volume fraction**

The mechanical performance of superalloys is controlled mainly by their crystalline microstructures. To be more specific, the excellent strength of superalloys is attributed largely to the presence of fine scale precipitates of ordered intermetallic phases in a ductile face-centered-cubic (FCC) solid solution matrix. Characteristics of the precipitate phase, such as volume fraction, average particle size, particle size distribution, particle morphology, and its stacking-fault properties, have been considered in the development of superalloys, and they have been treated as key factors for improving mechanical properties. For example, heat treatments have been developed to obtain optimal mechanical performance by controlling the particle size distribution, the volume fractions of secondary and tertiary precipitates, and regular or irregular morphologies of particles. While an intermediate particle size is related to peak strength, larger particles are associated with better performances of work hardening and fatigue resistance. Particle size can be controlled by the aging process, and the deformation process moves from particle shearing to Orowan looping. Average particle size generally determines an alloy’s properties when the width of the particle size distribution peak is narrow.
However, in many cases when the width of the peak is no longer narrow or when multiple peaks exist, the particle size distribution also controls the performance of the alloy, such as its yield strength and creep resistance. For example, a bimodal distribution is believed to provide a better combination of various mechanical properties than a unimodal distribution. For example, secondary particles enhance strength through Orowan looping and work hardening. At the same time, tertiary particles provide friction forces that increase both yield strength and creep resistance.

In addition to particle size distribution, particle volume fraction also controls deformation processes, including particle shearing and looping. For example, while the optimal volume fraction improves the strength of the alloy as well as creep resistance, extremely high volume fractions cause brittleness. Similar to the particle size, volume fractions of secondary and tertiary particles were considered separately, since they make different contributions to the yield strength and other properties of the alloy. Characterization of the volume fraction of particles requires digitization of the scanning electron microscope (SEM) or Transmission electron microscopy (TEM) pictures.

The characterized volume fraction and particle size always are used as inputs to the predictive models, which provide insight concerning how the performance of the alloy can be improved by changing the processing methods.

1.3. **Morphology and elastic energy of the precipitate**

Unlike volume fraction and particle size, which mainly control the averaged deformation behavior of the alloy, the morphology of the precipitate is a feature that controls both the
averaged and the local behaviors during deformation. It is believed that the morphology of the precipitate depends significantly on the crystalline misfit between the precipitate and the matrix. For example, the L1\textsubscript{2} structure has a smaller lattice parameter than the FCC matrix in the Ni-based superalloy. As a result, when a particle with L1\textsubscript{2} structure is embedded in an FCC matrix, elastic distortion occurs in both the particle and the matrix. The lengths of the atomic bonds vary across the particle boundary, which causes misfit strain. The appearance of misfit strain introduces an additional internal energy term, i.e., misfit elastic energy, to the total energy of the system. At the same time, misfit elastic energy decides the morphology of the particle. For example, for an L1\textsubscript{2} particle in an FCC matrix, spherical particle morphology is created when the elastic constants are isotropic, and rounded-cube particle morphology is obtained when the elastic constants are anisotropic. Both spherical and rounded-cube morphologies contain a symmetric operator, such as 3-fold rotational symmetry. When the crystalline structure of a particle has less symmetry, such as D0\textsubscript{22} (body-centered tetragonal), the misfit strain is anisotropic, and the particle’s morphology should represent this low symmetry. For a D0\textsubscript{22} particle in an FCC matrix, the morphology is disk-like in order to reduce the misfit elastic energy along the elongation axis. Since the tetragonal elongation can be expanded along any of the three <100> directions, there are three variants of the D0\textsubscript{22} structure, and they have been confirmed by TEM observations [2].

When multiple precipitate phases exist, the elastic interaction between the different precipitates causes more complex morphology, for example, composite particles. In
Chapter 3, we discuss the formation of composite particles in terms of elastic energy. Our simulation showed that the total elastic energy was reduced significantly by creating a hamburger-like or a cage-like morphology. The misfit strain fields of the $\gamma'$ and $\gamma''$ phases compensate for each other, and a spatial correlation between the $\gamma'$ and $\gamma''$ phases is preferred energetically. In contrast, improper composite morphology could be formed if an incorrect spatial relationship is created. The existence of an improper configuration was indeed a result of the reduction of spatial symmetry, which was due to the low symmetry of the $\gamma''$ misfit strain field.

In Chapter 3, the interactions between dislocation and misfit strain field are simulated by the phase-field deformation package. For the $\gamma''$ phase, due to the low symmetry of misfit strain field, the interactions between a given dislocation and different variants show different signs and magnitudes. As a result, a microstructure with $\gamma''$ particles displays anisotropy of plastic deformation whereas superalloys, which only have $\gamma'$ particles and any full dislocation is equivalent, experience identical particle shearing friction.

1.4. **Stacking fault of precipitate**

The precipitate consists of intermetallic phases, for example, $\gamma'$ (nickel-aluminum phase, L1$_2$, cubic) in nickel-base superalloys (such as ME 3 and Rene 88DT), and both $\gamma'$ and $\gamma''$ (nickel-niobium phase, DO$_{22}$, tetragonal) in nickel-iron-base superalloys (such as IN718 and IN706) have complex crystal structures and lower symmetry than the FCC matrix. As a result, many different deformation mechanisms are expected in the $\gamma'$ phase, i.e., APB, complex stacking fault (CSF), and superlattice intrinsic stacking fault (SISF). Initially,
the investigations were conducted mainly via electron microscopy characterization, but lately a combination of experimental characterizations and computer simulations has been used. For the $\gamma'$ phase in the nickel-based superalloys, for example, in addition to anti-phase domain boundary (APB) shearing [3], which occurs at relatively low temperatures and high stresses [4-11], other stresses have been observed at intermediate stress levels and temperature ranges that coincide with the service conditions of turbine disks [10]. These stresses include superlattice intrinsic stacking-fault (SISF) shearing, isolated superlattice-extrinsic-stacking-fault (SESF) shearing [3, 9, 12-15], microtwin [8, 9, 16-18], and stacking-fault ribbon shearing [11, 19].

Stacking-fault energy in the precipitate phase is a strong function of the crystalline structure, chemical composition, and service temperature. Systematic investigations have shown that structure with lower symmetry tends to possess higher stacking-fault energy. For example, a $1/6<112>$-type dislocation creates low energetic intrinsic stacking fault (ISF) in the matrix while there is high energetic CSF in both $L1_2$ and $D0_{22}$ structures. Experimental and theoretical works have shown that the stacking-fault energies of these structures are 20 mJ/m$^2$ (ISF in the matrix) and 221 mJ/m$^2$ (CSF in $L1_2$) [20]. At the same time, the space groups of FCC, $L1_2$, and $D0_{22}$ structures are Fm-3m, Pm-3m, and I4/mmm, respectively. The symmetry of an FCC structure is higher than that of $L1_2$ and $D0_{22}$ structures, and there is a strong correlation between the degree of symmetry and the stacking-fault energy.
Stacking-fault energy also is controlled by chemical composition. According to previous work by Michael Titus [21], the chemical dependence of APB energy displays a mixture relationship. In Ni-based and Co-based superalloys, APB energy is relatively higher. In the mixture case (CoNi-based), APB energy is lower. However, SISF energy varies monotonously as a function of composition according to TEM and theoretical analysis. These experimental observations indicate that there is no universal law concerning how energy varies with composition. The lack of a generality makes it very complex to predict the shearing mechanism. A database of stacking-fault energies for every composition is required to map the relationship between composition and the properties of the alloy. For example, we must know the relationship between Co composition in a Ni-based superalloy and its yield strength/creep resistance. The development of such a database will be extremely time-consuming, and it is beyond the scope of this work. In our work, for alloys with only a γ’ phase precipitate, we chose three compositions with well-evaluated stacking-fault energies. For 718-type alloy with both γ’ and γ” precipitates, the density-functional-theory (DFT) approach was used to calculate the stacking-fault energy and the structure of the γ” (D0_{22}) phase. To simplify the process, we assumed that the stacking-fault energy of the γ’ phase was the same as that in the Ni-based superalloy.

**Stacking-fault energy as a function of temperature**

In addition to crystalline structure and chemical composition, stacking-fault energy also is controlled by the service temperature. Currently, due to the complexity caused by structural and vibrational entropies, a direct *ab initio* calculation of stacking-fault energy
at a finite temperature is still challenging in terms of time and memory costs.

Alternatively, the thermodynamic approach, the mean-field approach, and experiments conducted with simple-structure crystals have been used to estimate the variance of stacking-fault energy with temperature.

First, based on a thermodynamic database, D. M. Collins et al. [22] indicated that there is a semi-linear relationship between stacking-fault energy and service temperature. In his work, APB\text{\{111\}} and APB\text{\{100\}} energies were investigated in the $\gamma'$ phase (Ni$_3$Al). The approach was based on modeling the interactions among the nearest atomic neighbors, and it was implemented by assuming that only the first nearest atomic neighbors dominate the APB energy. This thermodynamic-based model was calibrated using the CALPHAD method. Figure 2 shows the relationship for the temperature range of 600 - 800 °C.

![Figure 2](image_url)

**Figure 2.** The temperature dependences of the (111)-type and the (100)-type APB energies in the $\gamma'$ phase (L1$_2$, Ni$_3$Al) of the Ni-based superalloy. This is a theoretic result which is based on a thermodynamic database and the calculated by D. M. Collins et al. [22].
In order to use this relationship in the yield strength model, a linear slope was obtained by fitting this expression:

\[ \Gamma_{APB,\gamma'} = \Gamma_{APB,R} \times (1 - (T_K - T_R) \times \eta_d) \]  

(1)

where \( \Gamma_{APB,\gamma'} \) is the APB energy \((J/m^2)\) of the \( \gamma' \) phase; \( \Gamma_{APB,R} \) is the APB energy at the reference temperature, which can be measured by using TEM or SEM; \( T_K \) is the service temperature in K; \( T_R \) is the reference temperature (K) at which APB energy is measured; and \( \eta_d \) is the dropping rate of APB energy, which is 2.95e-4 1/K according to the calculation in the literature [22].

In addition to the thermodynamic-based model, another approach for estimating the temperature dependence of stacking-fault energy is based on the mean-field theory proposed by A.G. Khachaturyan [23]. According to this theory, stacking-fault energy decreases linearly at low and intermediate temperatures, which is the same result that was calculated by the thermodynamic-based approach in Collins’ work [22]. However, at a high-temperature range, stacking-fault energy decreases dramatically, as shown in Figure 3.
Figure 3: The temperature dependences of the stacking-fault energy in the L1$_2$ phase. This is a theoretic result which is based on the mean-field approach by A.G. Khachaturyan [23].

This dramatic decrease is due to the order-disorder transition, which is apparent in this mean-field approach. According to Fan’s calculation, the transformation temperatures of the γ” and γ’ phases in IN718 are both close to 1708 K (2615 °F) [24]. Above the critical temperature of 1708 K, which can be viewed as the order-disorder critical temperature, the chemical order of the L1$_2$ structure gradually disappears, and a cubic→FCC transition reduces the stacking-fault energy. As has been discussed previously, the DFT calculation and the experimental measurements showed that the higher structural symmetry implies the lower stacking-fault energy. Since the order parameter of the crystal structure
decreases as the temperature increases, the higher service temperature implies the lower stacking-fault energy.

In an experiment conducted by T. Kruml et al. in 1997 [25], in a Ni$_3$(Al, Hf) crystal, both the early stage of the linear decrement and the late stage of fast dropping were confirmed, as shown in Figure 4. Below 600 K, the dropping rate can be described as having a slope of approximately -0.07 mJ/(m$^2$K). Above 600 K, the dropping rate obviously was greater. In Chapter 5, the non-linearity of stacking-fault energy is used when fitting the yield strength model with the experimental yield strength of 718-type superalloy.

![Figure 4](image)

Figure 4. The temperature dependences of the APB energy in the γ' phase (L1$_2$, Ni$_3$(Al, Hf)). This is an experimental result [25]. When temperature > 600K, there is a fast-dropping of the APB energy.

For the L1$_2$ phase, we simply used the relationship in Figure 2, followed by rescaling the APB energy at room temperature to 172 mJ/m$^2$ [20] based on the experimental results obtained for the Ni-based superalloy. Actually, the effect of γ' hardening was trivial.
compared with the γ" phase, and a simple linear temperature dependence is adequate for the development of a simplified model.

1.5. **Orowan looping of precipitate**

In addition to the shearing process of the precipitate’s particles, Orowan looping is another significant deformation mechanism in a superalloy. Orowan looping occurs when the inter-particle distance (channel width) is wide, allowing dislocations to penetrate through the matrix. In microstructures with spherical particles, the width of the channel is calculated simply by subtracting the particle’s center distance by the particle’s radius. For microstructures with complex particle morphology and regular spatial arrangement, such as an elliptical precipitate, analytic expressions of the channel’s width already have been deduced \[26\] when the particle size is uniform and the spatial arrangement is regular and periodic. For example, elliptical particles appear in a triangular arrangement in Figure 5.

![Diagram of elliptical particles in a triangular arrangement](image)

Figure 5: The spatial arrangement of ellipse particles which is applied in the inter-particle distance calculation by M.R. Ahmadi \[26\]. A periodic triangular array is assumed.
In a real microstructure, the spatial distribution of particles is always irregular, and the size distribution can be extremely wide. However, as will be shown in Chapter 5, in a microstructure with a realistic particle size distribution and spatial distribution, the expression for elliptical particles still stands, while an acceptable error exists.

When the channel’s width \((Ch)\) is known, a classic expression of strength increment by line tension and the force balance on the dislocation line are expressed by the following equations:

\[
\Delta \tau_{LT} = \frac{Gb}{2\pi Ch} \left[ \frac{1 + 3\nu \sin^2 \theta}{1 - \nu} \right] \ln \left( \frac{Ch}{b} \right) \quad (2)
\]

\[
\Delta \tau_c = M \Delta \tau_{LT} + \Delta \tau_{LS} + \Delta \tau_{HP} \quad (3)
\]

where \(\Delta \tau_c\) is the critical stress of dislocation movement in a polycrystal, \(M\) is Taylor’s factor, \(\tau_{LT}\) is the strength increment due to line tension in a single crystal, \(\Delta \tau_{LS}\) is the lattice friction in a polycrystal, and \(\Delta \tau_{HP}\) is the Hall-Petch effect. In the expression of line tension strength, \(G\) is the shear modulus, \(Ch\) is the channel’s width, \(\nu\) is Poisson’s ratio, and \(\theta\) is the angle between Burgers vector and the direction of the dislocation line.

According to this expression, the critical stress of dislocation movement decreases with as the width of the channel increases when other parameters, such as shear modulus and lattice friction, are fixed.

In this above expression, critical resolved shear stress (CRSS) is calculated by using the average width of the channel. This approach has two implications. The first is that the width of the channel almost could be uniform. When dislocation movement can be activated in an average channel width, it can be activated in almost all of the channels.
Another implication is that dislocation source, such as Frank-Read source, could be distributed uniformly throughout the crystal.

In addition to the above expression, which uses the average width of the channel, CRSS also can be determined by searching penetrate pathways. This approach implies that dislocation sources are rare in a crystal or that they are concentrated only at the grain boundaries. As a result, even if the average width of the channel is large, percolation of dislocation is not guaranteed. Dislocation could be stopped completely by local, narrow channels if the narrow channels form a forbidden zone. In this case, the stress level that activates a percolation represents the CRSS of Orowan looping. In Chapter 5, an approach for simulating percolation is developed to calculate the active area of Orowan looping.

For a given microstructure, the critical stress of Orowan looping also is a function of service temperature. In addition to the temperature dependence of the shear modulus, the temperature dependence of lattice friction has been investigated in many experiments and calculations. For example, Figure 6 [27] shows the lattice friction in the Ni-based alloy.

The following expression in Ni-13.1Cr is used in the yield strength model in Chapter 5:

\[ \Delta \tau_{LS} = Sp_1 \times T_k + Sp_2 \]  

where \( Sp_1 = -0.0377 \text{ Ksi/K} \), \( Sp_2 = 39.15 \text{ Ksi} \), and \( T_k \) is the temperature in K.
1.6. Transition from shearing to looping

The transition from particle shearing to looping occurs in almost any alloy hardened by precipitate. For example, in Figure 7, the yield strength is plotted as a function of aging time [28]. In this example, the peak yield strength is achieved when the particle size is intermediate and the particle volume fraction is assumed to be invariant. The transition occurs at the peak where shearing and looping mechanisms become equally active. In a realistic case, an optimal combination of alloy properties should be achieved. For example, by controlling the heat treatment procedure, chemical composition, and mechanical processing, an optimal microstructure is generated with over-peak strength and desired fatigue resistance. In Chapter 5, the yield strength of 718-type superalloy is predicted with several different averages of particle size.
In terms of the internal energy of a material, the transition results from competition between the stacking-fault energy and line tension. When the width of the channel is narrow, dislocation will be curved significantly before passing through inter-particle spaces, which significantly increases line energy and, consequently, the CRSS of Orowan looping. If the particle size is small, the curvature of the dislocation segments on the particle boundary is large. In this case, the reduction in line energy will be significantly larger than the increment of stacking-fault energy if shearing occurs, and shearing will be preferred energetically.

However, when the channel is wide, dislocation can percolate easily through the matrix, while the curved dislocation line fraction is small. Meanwhile, for a microstructure that has larger particle size, the curvature on the particle boundary is low, and particle

Figure 7. The particle-size-distribution dependence of the yield strength according to the theoretic calculations [28]. The average particle size increases with the aging time.
shearing is less likely to occur. As a result, when the channel is wide and particle size is large, CRSS of shearing will be relatively higher than that of Orowan looping.

At the transition state, where either particle size or channel width is intermediate, the numerical simulations in Chapters 3 and 5 display a combination of shearing and looping.

In a much simpler case, i.e., when both the particle size distribution and the channel’s width distribution are narrow, by applying the CRSS expression as follows:

$$d\tau = \Delta \tau_L - \Delta \tau_S$$  \hspace{1cm} (5)

$$\Delta \tau_S = \Delta \tau_{s.f.c} - \Delta \tau_{s.f.a} + \Delta \tau_{res.L}$$  \hspace{1cm} (6)

where $d\tau$ is the difference in strength between particle looping and shearing, $\Delta \tau_L$ is the strength of particle looping, $\Delta \tau_S$ is the strength of particle shearing, $\Delta \tau_{s.f.c}$ is the strength increment by stacking-fault creation, $\Delta \tau_{s.f.a}$ is the strength decrement by stacking-fault annihilation, and $\Delta \tau_{res.L}$ is the looping strength increment related to residual dislocations, which are discussed in Chapter 5. When $d\tau < 0$, the looping mechanism tends to be active. When $d\tau > 0$, the shearing mechanism is preferred.

In Chapter 5, an analytic model based on the above equations is developed in order to determine how the shearing and looping populations vary with heat treatment and chemistry. These equations were modified in order to consider proper dislocation configuration and stacking-fault transformation. Proper dislocation is revealed by both TEM observations and DFT-based phase field simulation. Also, our work indicated that the aspect ratio of the $\gamma''$ particles and the temperature dependences of physical parameters also control the transition from shearing to looping. The shearing vs. looping
population is determined individually for each variant of $\gamma''$ particles. This consideration is necessary since the three-fold axis is broken on the (111) crystalline plane of the $\gamma''$ phase. As will be shown, a full dislocation will not create an equivalent stacking fault inside the different $\gamma''$ variants, and the shearing mechanisms are different.

For the $\gamma'$ phase, all of the particles are assumed to be sheared in this model. This is a reasonable assumption because 1) the stacking-fault energy of $\gamma'$ is relatively low and 2) their particle size is small.

The shearing vs. looping map is used as an input parameter of the fast-acting, yield-strength model, which is calibrated with experimental yield strength data. The relationship between yield strength and other physical parameters is largely represented through shearing vs. looping. Shearing vs. looping relies on several physical parameters, such as shear modulus, stacking-fault energy, volume fraction, particle size, aspect ratio, and lattice friction.

1.7. Dislocation configurations in superalloys

In superalloys, the dislocation configurations determine how precipitate and dislocation interact [29], and, consequently, they control the yield strength and creep rate of superalloys. Extensive research has been done on measuring dislocation configurations in Ni-based superalloys with $\gamma/\gamma'$ microstructure. However, only recently, some high-resolution studies were performed to determine the detailed dislocation configurations for the 718-type superalloy in a deformed microstructure [30].
According to the previous understanding, full dislocation pair and quadruplet [2, 4, 8, 31-37] are believed to be associated with the APB hardening in 718-type superalloy [32, 38, 39], since the $1/2<110>$ pair or quadruplet restores the perfect stacking sequence of the $\gamma''$ phase. As a result, yield strength was thought to result from the creation of an APB ribbon, and many models have been developed and tested to predict the increment of critical resolved shear stress (CRSS) [4, 39, 40] based on APB energy and work hardening.

However, the above guess is not supported by recent experimental observations. TEM measurements have shown how the low symmetric crystalline structure of the $\gamma''$ phase is associated with the complex dislocation structure, for example, the $<112>$ type dislocation.

![Figure 8. The shearing mechanism of the $\gamma'$ particle by an $<112>$-type dislocation group [10]. The deformation process firstly creates SISF area which is later consumed by the following APB and SESF. The final debris of this deformation process is an SESF whose formation requires the chemical re-ordering.](image)
Indeed, the $<112>$-type dislocation group already has been observed extensively in superalloys with $\gamma/\gamma'$ microstructure and recently in IN718. In Figure 8, 9, and 10, a classic explanation of the $<112>$ type dislocation group is provided [11, 19]. Several stacking-fault ribbons are formed in the $\gamma/\gamma'$ microstructure, and the re-ordering process triggers extrinsic stacking fault formation.

Figure 9. TEM picture of an (111) cross section sheared by the $<112>$ type dislocation group in the TMS-82+ superalloy. Both intrinsic (SISF) and extrinsic (SESF) faults are observed. [18]

Figure 10: A phase-field simulation revealed the dislocation core structure of the $<112>$ type dislocation group which has already interacted with a $\gamma'$ particle. Chemical re-ordering was not considered in this simulation. The SISF, APB, and CSF appear as the intermediate stacking ribbons of the deformation process. [18]
In this work, we will show that the $<112>$ type of dislocation is crucial when we offer our explanation of the dominant hardening mechanisms in 718-type superalloys. Also, the generality of the $<112>$ type dislocation is discussed in the absence of chemical re-ordering.

In Chapter 3, the $<112>$-type dominant configuration is investigated by applying DFT-based phase field simulation. The phase-field deformation simulation package predicts temporal evolution of dislocation and stacking fault. The configuration of the final stacking fault is characterized, and histogram plots are provided to show the distribution of debris. Our results show that the $<112>$-type dislocation group is related to the deformed microstructure observed by TEM. The $<112>$ dislocation and stacking-fault configuration are used later in the fast-acting, yield-strength model in Chapter 5.

1.8. Generalize-stacking-fault (GSF) potential surface

Currently, direct experimental measurement of stacking-fault energy in the $\gamma''$ phase is not available, since any stable single crystal of D0$_{22}$ structure with the composition of the $\gamma''$ phase in 718-type superalloy is not available. Alternatively, DFT method is applied in Chapter 2 to calculate 0K stacking-fault energy. Energy at finite temperature is obtained by scaling the stacking-fault energy.

Both structural and energetic information of stacking faults can be represented by a general stacking fault (GSF) potential surface [10, 41-43] which describes the stacking-fault energy as a function of arbitrary displacement vector $f$. It is defined as:
\[ \gamma(f) = \frac{(E(f) - E_0)}{S} \]

where \( E \) is the crystalline energy of the structure with stacking fault, \( E_0 \) is the perfect crystalline energy, and \( S \) is the stacking fault area. For a GSF-surface on (111) plane, the in-plane displacement is described by vector \( f \), which is the linear combination of \( f_1 = a/2[10-1] \) and \( f_2 = a/3[-12-1] \). The local minimum on the GSF-surface correspond the stable/metastable stacking faults. [11]

Figure 11. A GSF surface of the \( \gamma' \) phase (L1_2, Ni_3Al) was calculated by fitting an analytic expression with the DFT calculations. [20]

The ab initio DFT method has been proved to be a reliable approach to calculating the crystalline energy and defect formation energy in many crystals [10, 42, 44]. But it can only model crystal with very limited numbers of atoms. As a result, although the original definition of GSF surface requires an infinite out-of-plane distance between stacking faults, the energy of periodic stacking fault is calculated as an approximation. In order to
estimate the stacking-fault energy as accurate as possible, supercell size is carefully
tested in order to isolated periodic stacking faults along the out-of-slip-plane direction.
According to previous calculations of GSF surface, 6-layer supercell is sufficient to
isolate periodic stacking faults [45]. In the perfect stacking sequence, atomic layers are
stacked according to the displacement vector which represents periodicity of defined
crystals. For example, in the Al FCC structure, a supercell containing six (111) atomic
layers is applied, where the perfect crystalline structure follows the a-b-c-a-b-c stacking
sequence. In L1₂ structure, a-b-c-a-b-c stacking sequence is also applied, while in D0₂₂
structure, an a-b-c-d-e-f-a sequence is necessary to represent the tetragonal symmetry of
the crystal. A stacking fault is created when the perfect sequence is disturbed. For
example, APB in L1₂ structure corresponds to an a-b-c-a-b-c-a-b-a sequence, when a
mirror plane is introduced to the stacking sequence.
In order to eliminate the normal stress along the out-of-plane direction, which should not
appear in the definition of GSF, atomic position relaxation which is out of stacking fault
plane is necessary. Such kind of relaxation can not be performed in the standard VASP
package [46, 47]. However, by following the package developed by S. Ogata[48], the
internal stress along [111] direction is properly relaxed.
Besides the number of (111) type atomic planes, in-slip-plane atom number also needs to
be well selected in order to improve calculation speed. At the same time, equidistance
grid is applied to sample the asymmetric unit of the GSF-surface. For γ and γ' phase, the
final GSF-surface is obtained by fitting an analytic expression with discrete DFT
results[49]. However, for γ'' phase, there is no literature about its analytic GSF surface expression due to its structural complexity related to low symmetry.

Instead of the analytical expression, in this work γ'' GSF-surface is obtained through spline interpolation method [39]. Interpolation is performed based on DFT results of sampling points. Additional computation effort is necessary when energy pathways of some special shearing directions are simulated. It will be shown in Chapter 3 that the DFT GSF surface is used to identify unstable stacking fault and to reveal stacking fault transformation. This stacking fault transformation is the key to explaining dislocation and stacking fault configurations observed in 718-type superalloy. Also, novel dislocation source is found to be related to this stacking fault transformation. A DFT-based phase field approach is developed to simulate stacking fault configuration and dislocation structure. Implementation of γ'' GSF surface in phase field simulation will be discussed in Chapter 3. Also, the DFT-version GSF surface is an input of fast-acting yield strength model in Chapter 5.

1.9. Microscopic phase field model of dislocation-particle interactions

The phase field method is an efficient approach to treat dislocation-precipitate interactions [50]. It describes dislocation loops as shear platelets characterized by non-conserved order parameter fields, \( \eta_p (r) \) (where \( p \) indicates the slip system and \( r \) is the spatial coordinate) [51]. In an FCC crystal the displacement on a glide plane can be expressed as a linear superposition of three Burgers vectors [52]:

\[
\mathbf{b} = \eta_1 \mathbf{b}_1 + \eta_2 \mathbf{b}_2 + \eta_3 \mathbf{b}_3
\]  

(8)
where \( \mathbf{b}_1 = 1/2[0\bar{1}1], \mathbf{b}_2 = 1/2[10\bar{1}], \mathbf{b}_3 = 1/2[\bar{1}10] \), \( \eta_1, \eta_2 \) and \( \eta_3 \) are the order parameters describing inelastic displacement magnitudes along the corresponding Burgers vectors. The stacking fault of a given Burgers vector \( \mathbf{b} \) can be found on the GSF potential surfaces. The eigenstrain associated with a dislocation with Burgers vector \( \mathbf{b}_p \) is:

\[
\varepsilon_{ij}^{\text{dist-p}} = \frac{\mathbf{m} \otimes \mathbf{b}_p + \mathbf{b}_p \otimes \mathbf{m}}{2d^{(111)}}
\]

(9)

where \( \mathbf{m} = \frac{\sqrt{2}}{3} [111] \) is the dislocation glide plane normal, \( \otimes \) denotes dyadic product, \( d^{(111)} \approx 0.208 \) \( \text{nm} \) is the \{111\} planes spacing in IN718 (the lattice parameter of the \( \gamma \) phase is \( a \approx 0.36 \) \( \text{nm} \)).

The time-evolution of an arbitrary dislocation configuration consisting of various dislocation loops is governed by the time-dependent Ginzburg-Landau (TDGL) equations [51, 53-55]

\[
\frac{\partial \eta_p}{\partial \tau} = -L_p \frac{\delta F}{\delta \eta_p} \quad p = 1, 2, 3
\]

(10)

where \( F \) is the total free energy of the system, \( L_p \) is the kinetic coefficient characterizing dislocation mobility and \( \tau \) is a reduced time. The activation of different deformation modes (for example: SISF shearing vs. APB shearing, shearing vs. looping, etc.) is determined by local interactions between precipitates and dislocations without any \textit{a priori} assumptions (such as a critical size of particles). Dislocation dissociation and reactions in different phases are controlled by the GSF potential surfaces, precipitate microstructures and applied stress.

The total free energy of the system consists of the crystalline energy [49, 51, 52], \( E^{\text{crystal}} \) (directly linked to the GSF energy), the gradient energy, \( E^{\text{grad}} \) (part of the core energy), and the elastic energy, \( E^{\text{elast}} \), which includes the work done by an applied stress:
\[ F = E^{\text{crystal}} + E^{\text{grad}} + E^{\text{elast}} \]  

(11)

For any specific slip plane, the crystalline energy is described by the GSF energy [50, 52]. The gradient energy term [49, 51], follows the gradient thermodynamics of non-uniform systems [56-58], appears naturally during limit transition from discrete to continuum [50, 59, 60]. The expression of the gradient energy term can be find in Ref. [49]:

\[ E^{\text{grad}} = \frac{\beta}{2} \sum_{p,q=1...3} \left[ m \times \nabla \eta_p \right] \cdot \left[ m \times \nabla \eta_q \right] \]

(12)

where \( m = \frac{\sqrt{2}}{3} [111] \) is the dislocation glide plane normal and \( \beta \) is the gradient energy coefficient. The elastic energy due to the presence of dislocations, external load and misfit stress of precipitates can be described by using Khachaturian's microelasticity theory [23, 61, 62]:

\[ E^{\text{elast}} = \frac{1}{2} \int \sum_{p,q=1...3} \frac{d^3k}{2\pi} B_{pq}(n) \eta_p(k) \eta_q^*(k) - \sigma_{ij}^{ex} \int \sum_{p=1...3} \varepsilon_{ij}^p \eta_p \, dV \]

(13)

where:

\[ B_{pq}(n) = \begin{cases} 0; & n = 0; \\ \frac{C_{ijkl}}{n_j n_k}; & n \neq 0 \end{cases} \]

(14)

for a stress-controlled (i.e., constant stress) boundary condition, \( \mathbf{k} \) is the reciprocal space vector and \( n = k/|k| \), \( \sigma_{ij}^{P} = C_{ijkl} \varepsilon_{ij}^p \varepsilon_{kl}^q - n_j \sigma_{ij}^{p} \Omega_{jk}^{-1}(n) \sigma_{kl}^q n_l \). The second term in Eq. (6) is the work done by an applied stress. Note that the coherency stress of the precipitates is not considered in the current study.
1.10. Physics-based yield-strength model

Besides empirical analysis, which is developed based on the statistics of experimental data, physics-based models [38, 41, 63] are required to calibrate empirical models and provide deep insight concerning the deformation process. In addition, physics-based models enable a top-down design approach [63], which accelerates alloy development in order to satisfy the ever-changing specific application requirements.

One of the major steps in developing a physics-based yield-strength model of a superalloy is to understand the dislocation configuration related to the precipitate. In the FCC matrix, the dislocation with Burgers vector of a/2<110> on the \{111\} plane restored the perfect stacking sequence and left no extra fault energy. Only extra surface energy is created at the material surface and can be ignored in a bulk material. As a result, it is easy for an a/2<110>-type, full dislocation to be active in the matrix, and there is no necessity for dislocations to create a group in order to move.

However, full dislocation always leaves a stacking fault inside the ordered precipitate phase. For example, in the L12 γ' precipitate, APB is left when any dislocation cuts through a perfect crystal [4, 29, 38]. Since APB always has much higher crystalline energy than that of the perfect stacking sequence, individual dislocation cutting is actually not energetically favorable. Dislocation shearing is only active when full dislocations with the same Burgers vector team up in pairs [8], creating an APB ribbon with limited width. After the second dislocation cuts through, a perfect stacking sequence is restored, and there is no extra fault energy left.
Creation of the APB ribbon introduces an increment of CRSS, which is called APB ribbon hardening. APB ribbon hardening or a similar mechanism exists in many alloys with precipitates, and the fault inside the ribbon is not always APB. For example, during the shearing by <112> type dislocation, APB, SISF, and SESF all form their own ribbon structures. Similar to APB hardening in the $\gamma'$ phase, the $\gamma''$ phase also can contribute to yield strength through the formation of a stacking-fault ribbon. For years, people thought that the fault structure in the ribbons of the $\gamma''$ phase also was APB. According to this understanding, there are two typical dislocation configurations associated with hardening, i.e., (1) pairs of full dislocation and (2) quadruplet dislocation. Configuration is considered in addition to pair since, for a given Burgers vector, only one variant of the $\gamma''$ phase can be restored by a pair of dislocations, while only quadruplet restores the perfect stacking sequence in the other two variants.

A typical analytical formula for calculating the increment of CRSS by the pair dislocations is [2]:

$$\Delta\tau = \left[ \frac{\Gamma_{\gamma''}}{2b} \left( \frac{4\gamma_{\gamma''} f_{\gamma''}}{\pi T} \left[ \frac{\sqrt{6} Rh}{3} \right]^{1/2} \right)^{1/2} - \beta f_{\gamma''} \right]$$

(15)

where $\Delta\tau$ is the CRSS increment due to APB ribbon, $\Gamma_{\gamma''}$ is the APB energy of the $\gamma''$ phase, $b$ is the length of Burgers vector, $a\sqrt{2}/2$, $f_{\gamma''}$ is the volume fraction of the $\gamma''$ phase, $T$ is dislocation line tension ($\sim \frac{1}{2} \mu b^2$ for an edge dislocation), and $\beta$ is the number fraction of $\gamma''$ particles for which the perfect-stacking-fault sequence is restored. In a
microstructure in which three variants of \( \gamma'' \) particles have the same number fraction, i.e., \( \beta = 1/3 \), \( R \) is the average radius, and \( h \) is the average half thickness of the \( \gamma'' \) particles.

The aspect ratio is represented by the relationship between \( R \) and \( h \).

Similar to the pair of dislocations, the dislocations in a quadruplet group share a common Burgers vector on the same slip plane. The dislocation quadruplet in D0\(_{22}\) is believed to be coupled by multiple APB ribbons, as is illustrated in Figure 12. In one of the variants, the ribbon sequence is ABP->perfect structure ->APB. In the other two variants, the ribbon sequence is expected to be ABP->APB->APB.

In terms of stacking-fault energy, 2/3 variants of the \( \gamma'' \) phase prefer the quadruplet group of dislocations. The analytical formula of CRSS increment by dislocations quadruplet is [2]:

\[
\Delta \tau = \left[ \frac{\Gamma_{\gamma'}}{4b} \left( \frac{4\Gamma_{\gamma'} f_{\gamma'}}{\pi T} \left[ \frac{\sqrt{\varepsilon_{\gamma'}} R}{3} \right]^{1/2} \right)^{1/2} - f_{\gamma''} \right]
\]

(16)

where the symbols have the same meanings as they have in the analytical formula that is used to calculate the CRSS increment by the dislocation pair.

Understanding of stacking-fault properties is the key to improving the physics-based, yield-strength model. In previous works, among all stacking faults of the \( \gamma'' \) phase in the 718-type superalloy, attention was paid only to APB hardening since the APB-type model already has been successful in \( \gamma/\gamma' \) microstructures. However, as is shown in Figure 12, the APB-type model in \( \gamma/\gamma'' \) microstructure has two basic assumptions [2]. The first assumption is that Burgers vector of every single dislocation in a group (such as pair
and quadruplet) is identical. After cutting by quadruplet, there is no high energetic debris inside the γʺ particles.

Figure 12. A TEM picture and a conceptual diagram which give one possible explanation of the dislocation configuration in the γʺ dominating superalloy (e.g., 718-type) [2].

Actually, the above assumption is not necessary, because dislocations with different Burgers vectors also can form an active group and leave a perfect stacking sequence inside the γʺ particles. For example, the following two combinations, i.e., (1) a/2[1-10] + a/2[0-11] = a/2[1-21] and (2) a/2[10-1] + a/2[1-10] + a/2[10-1], also restore the perfect stacking sequence of the γʺ phase. In addition, according to recent TEM observations, the <110> type dislocation group has not been confirmed within the deformed IN718 microstructure.

The second assumption of the APB-type models is that every full dislocation generates APB in any variant of γ" precipitate. This could be a reasonable approximation only
when three-fold rotational symmetry holds. However, as is discussed in Chapter 2, APB-like stacking fault and APB are totally different structures in terms of symmetry and have significantly different energies. Also, the model is not able to consider any unstable stacking fault or stacking-fault transformation, which is highly possible in particles with significantly lower symmetry than that of the matrix.

Besides the improper assumptions mentioned above, classic APB-type models cannot consider the dislocation dissociation or partial dislocation inside the \( \gamma'' \) particle. Actually, that is the reason that stacking-fault ribbons (SISF, CSF, ISF) are hard to model using the old approach. In the L\( _2 \) structure and matrix, dislocation dissociation has been found to reduce CRSS of shearing by changing the deformation pathway and avoid the high energetic state. The deformation energy pathway is chosen to have a lower barrier than the undissociated, full-dislocation pathway. As a result, dislocation dissociation in the matrix and L\( _2 \) particles enhance the activation of full dislocation, and a stacking-fault ribbon with lower energy is created instead of an APB ribbon [64]. In the matrix, an ISF ribbon can be formed that connects leading and trailing partials. In the L\( _2 \) structure, the SISF ribbon connects the 1/3<112> super-dislocation and the 1/6<112> partial dislocation.

Possible dissociations in the D\( _{022} \) structure are discussed in Chapter 3, which provide a basis for an improved physics-based, yield-strength model. Then, the stacking fault and dislocation configurations in the analytical expressions must be modified. Indeed, if it is easy for dislocation dissociation to be active, it is natural to expect the 1/3<112> type
super-dislocation or another $<112>$ type dislocation group, as happened with the L1$_2$
particle. In recent TEM observations, $<112>$ type dislocations were dominant in
superalloy IN718 in which the $\gamma''$ phase has a larger volume fraction than the $\gamma'$ phase.
In addition to dislocation dissociation, there is another way to explain the $<112>$
dislocation observed in the $\gamma''$ phase dominating alloys. As discussed in Chapter 2, there
are unstable stacking faults in D0$_{22}$, such as CSF and APB-like faults. If these
configurations are formed by the input dislocation from the matrix, they will
spontaneously transform to the nearest stable/metastable stacking fault, such as a perfect
stacking sequence or ISF. Accompanied by the transformation, there will be a partial
dislocation emissions, which is a novel source of dislocation, which increases dislocation
density inside a crystal. It could explain the observed $<112>$-type dislocation loops around
$\gamma''$-phase particles.
Partial dislocation emissions ultimately will change the stacking-fault configuration in the
deformed microstructure. As a result, the explanation of the observed stacking fault will
be more complex in the $\gamma'/\gamma''$ microstructure than in the $\gamma'/\gamma'$ microstructure. For example,
in the L1$_2$ structure, if we know all of the dislocation cuts through the particle, then an
APB is expected to be debris. However, in the D0$_{22}$ structure, if a full dislocation from
the matrix shears the particle, then APB can be formed in one variant. But, in the other
two variants, APB-like fault is formed, which is unstable and will transform to nearby
stable structures. Consequently, the displacement vector of final stacking-fault formation
will be different from Burgers vector of input dislocation. In the physics-based, yield-
strength model, it is important to consider the final stacking-fault configuration related to
dislocation emissions, since the stacking-fault transformation releases the final stacking-
fault energy and reduces CRSS. To do this, we must understand the transition pathway
from DFT and phase-field simulations. Also, the final stacking-fault configuration, which
is modified by partial emission, will help explain the measured stacking configuration in
718-type superalloys.
A new model must be developed in order to correctly describe stacking-fault ribbon,
dislocation dissociation, and partial dislocation emissions. In Chapter 5, a mathematical
model is shown, and a CRSS expression with a term of partial dislocation emissions is
obtained. Also, the model is modified so that other stacking-faults, such as CSF, SISF,
APB-like fault, and ISF, can be considered.
Chapter 2: Generalized-Stacking-Fault (GSF) Potential Surfaces of Precipitate Phases

The $\gamma''$ phase has a crystal structure with the lower symmetry than that of the $\gamma'$ phase, which means that more complicated deformation mechanisms are expected. However, up to now only the APB hardening has been considered, and the APB energy is the only material parameter related to the shearing that appears in the constitutive descriptions of the yield strength for the 718-type superalloy [2]. This is an obviously inadequate assumption considering the recent TEM characterization of the deformation microstructures in a crept IN718 single crystal [30, 65, 66]. In that observation, neither APBs in $\gamma''$ particles nor $<011>$ type dislocation group exists in the matrix.

Figure 13. The 3-D diagrams of the crystalline structures of the $\gamma$ (FCC, Ni), $\gamma'$ ($L1_2$, Ni$_3$Al) and $\gamma''$ ($D0_{22}$, Ni$_3$Nb) phases.
Meanwhile, both the experimental characterizations and the *ab initio* calculations \([64, 67-69]\) of the plastic deformation in a similar crystal of Ni\(_3\)V revealed several new types of stacking faults that are absent in the L1\(_2\). The Ni\(_3\)V single crystal has also a D\(0_{22}\) structure. In the D\(0_{22}\) due to the absence of the 3-fold rotational symmetry, for example, an APB-like stacking fault (APB\(_{\|}\)) \([68]\) is discovered. The APB-like structure inherits the Burgers vector of the APB in the intermetallic phases with a cubic symmetry, while several mirror plane operations are lost. In addition, in the D\(0_{22}\) an intrinsic stacking fault (ISF) \([64]\) is identified, and the ISF has low stacking-fault energy which is similar to the case in the matrix. Several ISFs on adjacent atomic planes is related with the SESF \([64]\) which is a precursor to the microtwin \([67]\) and has been observed widely in the Ni\(_3\)V single crystal.

The shearing strength and pathway of a crystal on a given crystallographic plane (i.e., the slip plane) are represented by the generalized-stacking-fault (GSF) potential surface \([70, 71]\). At the same time, because the detailed shearing mechanisms of the precipitates depend also on particle size, morphology, and spatial arrangement, the DFT calculation alone is hard to achieve the desired length scale. As a result, a large-scale simulation approach is required to calculate the temporal evaluation of the deformation process. The microscopic phase field model \([50, 72]\), bridges the *ab initio* calculations and the mesoscale modeling of dislocation-precipitate interactions, including the dislocation dissociation, the teaming up of dislocations, and the stacking fault formation \([11, 18, 43, 49-52, 73, 74]\).
In this study, we calculated the GSF energy surface on \{111\} slip plane of the $\gamma''$ phase using the *ab initio* calculations. Note that the Miller indices for both crystallographic directions and planes are represented on the basis of the $\gamma$ matrix phase (FCC) for convenience.

### 2.1. Fundamental properties of $\gamma''$ phase from DFT calculation

The lattice parameters and elastic constants at 0K are calculated by using DFT method. The results of these parameters are listed in Table 1. The lattice parameter calculations were performed by relaxing the shape and volume of the unit cell while fixing the symmetry of the D0$_{22}$ structure. By fitting the relationship between the potential energy and the strain tensor, the stiffness tensor is calculated as the fitting parameter of the following equations:

$$ U = \frac{1}{2} \sum C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \quad (17) $$

Where $U$ is the total potential energy, $C_{ijkl}$ is the 4$^{\text{th}}$ order tensor of stiffness, and $\varepsilon_{ij}$ is the strain tensor.

By calculating the total free energy as a function of volumetric strain and fitting the following relationship by Birch-Murnaghan EOS, the bulk modulus is obtained:

$$ E(V) = E_0 + \frac{9V_0B_0}{16} \left\{ \left( \frac{V_0}{V} \right)^\frac{2}{3} - 1 \right\}^3 B'_0 + \left\{ \left( \frac{V_0}{V} \right)^\frac{2}{3} - 1 \right\}^2 \left\{ 6 - 4 \left( \frac{V_0}{V} \right)^2 \right\} \quad (18) $$

Where $E(V)$ is the total internal energy, $E_0$ is the internal energy in the absence of external pressure, $V_0$ is the reference volume, $V$ is the volume under pressure. $B_0$ is the
bulk modulus and $B'_0 = \left(\frac{\partial B_0}{\partial P}\right)_{P=0}$, which are determined as fitting parameters. This is a
standard and accurate approach to calculating bulk modulus through DFT method.

According to the table, the calculated lattice parameters $a$ and $c$ agree well with the
theoretic results in the literature [75-77]. The calculations have been done with all the
available potentials in VASP. The elastic tensor which is calculated by using PAW-GGA
also agrees well with the values reported in the literature [76, 77]. Additionally, the
calculated magnetic moments are always zero, which is consistent with the results
reported in D. Connetable [78] and W.T. Geng [79]'s works for the same crystal.

<table>
<thead>
<tr>
<th>Method</th>
<th>a(Å)</th>
<th>c(Å)</th>
<th>C1</th>
<th>C1</th>
<th>C1</th>
<th>C33</th>
<th>C44</th>
<th>C66</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp.[75-77]</td>
<td>3.57 (LDA)</td>
<td>7.35(LDA)</td>
<td>288</td>
<td>188</td>
<td>162</td>
<td>299</td>
<td>115</td>
<td>104</td>
</tr>
<tr>
<td></td>
<td>3.65 (GGA)</td>
<td>7.50(GGA)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.62 (EXP.)</td>
<td>7.41 (EXP.)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LDA</td>
<td>3.58</td>
<td>7.33</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GGA</td>
<td>3.66</td>
<td>7.51</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PAW</td>
<td>3.57</td>
<td>7.31</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PAW-GGA</td>
<td>3.66</td>
<td>7.48</td>
<td>283</td>
<td>180</td>
<td>165</td>
<td>292</td>
<td>112</td>
<td>102</td>
</tr>
<tr>
<td>PAW-PBE</td>
<td>3.66</td>
<td>7.48</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 1. The lattice parameters and elastic modulus (GPa) of \(\gamma''\) phase.

What is more, according to the criteria of mechanical stability in the tetragonal phase [80, 81]:

\[
C_{11} - C_{12} > 0, C_{11} + C_{33} - 3C_{13} > 0, \\
2(C_{11} + C_{12}) + C_{33} + 4C_{13} > 0 \\
C_{11} > 0, C_{33} > 0, C_{44} > 0, C_{66} > 0
\]  \(19\)
As a result, the D0$_{22}$ supercell modeled in our work is mechanically stable.

### 2.2. Stacking faults in $\gamma''$ phase

Figure 14. The six-layer supercells of a DO$_{22}$ structure containing various stacking faults.

In Figure 14, the stacking faults in a D0$_{22}$ structure are plotted inside 6-layer supercells. The view direction is along [-110] and [-1-12]. These supercell structures are used when performing the DFT calculations of the SF energies. In each supercell, an SF appears periodically in every 6th atomic layer which satisfies the periodic boundary condition required by the DFT approach. What is more, Figure 14 corresponds to TEM images where SF displacements are determined by the Burgers circuit.
Figure 15. The atomistic configurations viewed along the [111] of a D0_{22} structure showing the APB, CSF, SISF, APB-like stacking fault, and CSF-like stacking fault. The black and blue dashed lines indicate the mirror planes.

In order to reveal and analyze the symmetry of stacking fault, an [111] view of the supercell structures is plotted in Figure 15. The intrinsic stacking faults, in which the planar displacements are constrained within only one atomic layer, are the focus of the current study. As a result, only two adjacent atomic layers are displayed to explain the relative displacement which defines a stacking fault. In the APB configuration (Figure 15
(b)), the Burgers vector of 1/2[-110] (the yellow arrow) causes a changing of nearest neighbor relationship. For example, the Nb atoms in the top layer become the nearest neighbors of the Nb atoms in the bottom atomic layer. When this displacement is repeated on more time, the perfect stacking sequence is restored. The restoration satisfies the definition of APB, which has been applied in the L1_2 structure.

In Figure 15(e), the Burgers vector of 1/2[01-1] will also change the nearest neighbor relationship. The displacement brings the Nb atoms in the top atomic layer to be the nearest neighbors of the Nb atoms in the bottom atomic layer. This nearest relationship is the same as the atomic configuration in APB. However, another aspect of the atomic configuration which is different from that of APB is shown in Figure 15(b), in terms of the structural symmetry and consequently the fault energy listed in Table 2. As a result, this stacking fault is named as APB-like stacking fault (or APB_{II}) instead of ABP,

following the convention which has been used in Ni_3V (D0_{22}) [64, 68, 69].

<table>
<thead>
<tr>
<th>Stacking fault</th>
<th>Displacement</th>
<th>Free energy (mJ/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ISF</td>
<td>1/6[11-2]</td>
<td>2.301</td>
</tr>
<tr>
<td>APB</td>
<td>1/2[-110]</td>
<td>592.1</td>
</tr>
<tr>
<td>SISF</td>
<td>1/3[-12-1]</td>
<td>613.6</td>
</tr>
<tr>
<td>CSF</td>
<td>1/6[-211]</td>
<td>697.9</td>
</tr>
<tr>
<td>APB-like stacking fault</td>
<td>1/2[01-1]</td>
<td>482.3</td>
</tr>
</tbody>
</table>

Table 2. The displacement vector and stacking fault energies.

Starting from APB-like stacking fault, the second 1/2[01-1] displacement vector cannot restore the perfect stacking sequence of a D0_{22} crystal. The lower symmetry of APB-like
stacking fault is represented by losing the mirror planes (blue and black dashed lines in Figure 15) perpendicular to the (111) plane. According to the calculation of GSF surface, the APB-like structure is not mechanically stable.

In Figure 15(d), an SISF (superlattice intrinsic stacking fault) structure is defined. Again, the definition follows the convention used in Ni₃V. It is created by the Burgers vector 1/3[-12-1], and only in terms of the Burgers vector, this configuration is similar with the SISF in L1₂ structure. However, the atomic configuration of SISF (D₀₂₂) is quite different from SISF (L₁₂), because the Nb atoms in the top atomic layer become the nearest neighbors of Nb atoms in the bottom atomic layer. In contrast, in SISF configuration in L₁₂ there is no first nearest neighbor with Al-Ni bond. As a result, strictly speaking, the SISF in D₀₂₂ should be called SISF-like.

In Figure 15(f), a CSF structure is reached by Burgers vector 1/6[-211]. Similar with the CSF in L₁₂ where the Al atoms in the top atomic layer becomes the nearest neighbors of Al atoms in the bottom atomic layer, in D₀₂₂ structure, the Nb atoms in the top atomic layer become the nearest neighbors of Nb atoms in the bottom atomic layer. The difference is that in D₀₂₂ the CSF is an intermediate state between perfect crystal and APB-like stacking fault instead of APB, due to the lack of 3-fold rotational symmetry in D₀₂₂. Again, it should be mentioned that APB and APB-like stacking fault are no longer equivalent in D₀₂₂.

Finally, an ISF is defined in Figure 15(c), where the atomic neighbor relationship is similar with that in ISF of FCC structure. The Burgers vector associated with ISF is
1/6[11-2], and the nearest neighbor relationship of any element in the faulted structure is unchanged. As a result, stacking-fault energy of ISF is ultra low (~2.3 mJ/m²) (Table 2). In contrast, the stacking fault energies of other structures in Table 2 are much higher because in these faults the nearest neighbor relationship is different from that of a perfect crystal.

2.3. GSF energy surface of γ'' phase from DFT calculation

In order to reveal the stacking fault stability, stacking-fault energy and energy barrier during deformation process, GSF energy surface is calculated in addition to the energy of special SFs. In Figure 16 the GSF surface landscape is plotted as a function of in-plane x- and y-displacements.

Figure 16. The generalized-stacking-fault (GSF) potential energy surface of the equivalent(111)γ plane in γ'' phase. The red-dashed box indicates the periodically repeating unit of the GSF-surface. The Burgers vectors of different faults (indicated by the arrows) are given in the legend. The blue arrow indicates the displacement along 1/2 [11-2]. The white arrow indicates the displacement along 1/2 [-110]. The yellow arrow indicates the displacement along 1/6[-110]. The green arrow indicates the displacement along 1/6[-12-1].
In order to reduce the computational cost (both time and memory cost), only 5x12 equal-distance grid is used to sample the asymmetric unit (within the red dashed box in Figure 16 on the GSF surface). Specific energy pathways are plotted by using the result of this calculation. These specific pathways are shown in Figure 17. The calculations follow the approach which has already been applied in the literature [48].

Figure 17. GSF energy landscapes along special deformation pathways: (a) along $\frac{1}{2} [11-2]$; (b) along [-110]; (c) along 1/6 [-211] (blue solid line) and 1/6 [-12-1] (red dashed line); (d) along 1/6 [-12-1] (blue solid line) and 1/6 [-211] (red dashed line).
As is shown in Table 2, ISF energy of $\gamma''$ phase is calculated to be $\sim$2.3 mJ/m$^2$.

Meanwhile, the energy barrier along the pathway toward ISF is $\sim$252 mJ/m$^2$, as is shown in Figure 17. This value is very close to the energy barrier along the pathway toward ISF in FCC(Ni) (269 mJ/m$^2$) which is also obtained by DFT approach [41]. The ultra low SF energy and relatively weak deformation barrier imply that a large amount of ISF can exist inside the $\gamma'/\gamma''$ microstructure, which will enhance the activation of SESF and microtwin, and induces a similarly deformed microstructure in Ni$_3$V(D0$_{22}$) single crystal [68].

2.4. Stability of stacking faults

In both $\gamma$ and $\gamma'$ phases, there is a necessary condition which should be satisfied when creating stable stacking fault (i.e., at a stable mechanical equilibrium): each atom must lay within a triangular depression created by the nearest-neighbor atoms in the two adjacent {111} atomic layers. All the stable stacking faults in these phases such as ISF, APB, CSF, and SISF satisfy this criterion. In $\gamma''$, however, as a consequence of its lower symmetry, GSF energy surface calculation reveals another necessary condition of stable stacking fault in addition to the triangular depression filling rule. This additional condition can be described as:

*In the two-atomic-layer stacking fault illustrations in Figure 15, the vertical mirror planes (indicated by the blue and black dashed lines) have to be preserved in a stable stacking fault.* In any unstable stacking fault these two mirror planes are lost, which causes the absence of local minima on the energy contour.
When this additional condition is also met, the displacements end up at local minima on the GSF energy surface, which include ISF, APB, and SISF. The mirror planes are lost in both CSF and APB-like fault and thus they are unstable. This instability is indicated by the specific energy pathways plotted in Figure 17. These unstable SFs must transform into nearby stable SFs. Accompanied with stacking fault transformation, new dislocation configurations are generated, which brings out challenges in identifying the operating deformation mechanisms of the $\gamma''$ phase. Also, the stacking fault transformation requires modification of existing yield strength models, in order to consider the novel dislocation structure and SF configuration and to predict the mechanical behavior of realistic engine components.

2.5. **GSF surface of $\gamma$ phase (L1$_2$ structure)**

For L1$_2$ structure, GSF potential surface on (111) plane should have a 3-fold axis and three mirror planes. An analytical GSF expression which represents these symmetry operations is applied:
\[ \Gamma(\eta_1, \eta_2) = c_0 + c_1 \left( \cos(\pi \eta_1) + \cos(\pi \eta_2) + \cos(\pi (\eta_1 - \eta_2)) \right) + c_2 \]
\[ \left( \cos(\pi (2 \eta_1 - \eta_2)) + \cos(\pi (\eta_1 + \eta_2)) \right) + c_3 \]
\[ + \cos(\pi (\eta_1 - 2 \eta_2))) + c_4 \]
\[ \left( \cos(2\pi \eta_1) + \cos(2\pi \eta_2) + \cos(2\pi (\eta_1 - \eta_2)) \right) + c_5 \]
\[ + \cos(\pi (3 \eta_1 - \eta_2)) + \cos(\pi (3 \eta_1 - \eta_2)) \]
\[ + \cos(\pi (2 \eta_1 + \eta_2)) + \cos(\pi (\eta_1 + 2 \eta_2)) \]
\[ + \cos(\pi (\eta_1 - 3 \eta_2)) + \cos(\pi (2 \eta_1 - 3 \eta_2)) \]
\[ + \cos(3\pi \eta_1) + \cos(3\pi \eta_2) + \cos(3\pi (\eta_1 - \eta_2)) \]
\[ + \cos(4\pi \eta_1) + \cos(4\pi \eta_2) + \cos(4\pi (\eta_1 - \eta_2)) \]
\[ + \cos(5\pi \eta_1) + \cos(5\pi \eta_2) + \cos(5\pi (\eta_1 - \eta_2)) \]
\[ + \cos(\eta_1) + \cos(\eta_2) + \cos(\eta_1) \]
\[ + \sin(\eta_1) + \sin(\eta_1 - \eta_2) \]
\[ + \sin(\eta_1 - \eta_2) + \sin(\eta_1) \]
\[ + \sin(\eta_1 + \eta_2) + \sin(\eta_1 + 2 \eta_2) \]
\[ + \sin(\eta_1 - \eta_2) + \sin(\eta_1 - 2 \eta_2) \]
\[ + \sin(\eta_1) + \sin(\eta_1 + \eta_2) \]
\[ + \sin(\eta_1 + \eta_2) + \sin(\eta_1 - 2 \eta_2) \]
\[ + \sin(3\eta_1) + \sin(3\eta_2) + \sin(3\eta_1 + \eta_2) \]
\[ + \sin(3\eta_2) \]
\[ + \sin(4\eta_1) + \sin(4\eta_2) + \sin(4\eta_1 + \eta_2) \]
\[ + \sin(4\eta_2) \]

(20)
Where \( c_i \) are undetermined parameters. \( \eta_1 \) and \( \eta_2 \) are order parameters which describes displacement field as has been mentioned in Chapter 1. Parameters in the expression are later obtained by fitting expression with data in Figure 18.

Figure 18. The composition dependence of the stacking fault energies. The data points are obtained for the Ni-based, Co-based and CoNi-based superalloys.

DFT and experiment only provide APB and SISF energies at specific compositions. The analytic expressions of APB and SISF with independent variable of composition follow the work by Michael Titus:

\[
\Gamma_{APB}(X_{Co}) = p_{APB,1} \times X_{Co}^2 + p_{APB,2} \times X_{Co} + p_{APB,3} \tag{21}
\]

\[
\Gamma_{SISF}(X_{Co}) = p_{SISF,1} \times X_{Co}^2 + p_{SISF,2} \times X_{Co} + p_{SISF,3} \tag{22}
\]

Where \( \Gamma_{APB} \) and \( \Gamma_{SISF} \) are APB energy and SISF energy in terms of mJ/m². \( X_{Co} \) is Co composition ranging from 0 to 1. For Ni-based superalloy, Co composition is assumed to be 0. In Co-based superalloy, \( X_{Co} \) is assumed to be 1. Co composition is assumed to be 0.5 in CoNi-based superalloy. The values of parameters are listed:

\[
p_{APB,1} = 400, \quad p_{APB,2} = -480, \quad p_{APB,3} = 240, \quad 47
\]
\[ p_{SISF,1} = 50, p_{SISF,2} = 25, p_{SISF,3} = 55 \]

Although APB and SISF energies are known, the parameters \( c_i \) in the GSF expression (totally 11 undetermined parameters) cannot be determined until more data points are available. Additional data points include CSF energy and barrier height between stable configurations. According to literature [20], the ratio between CSF and APB energies can be estimated as:

\[
\frac{\gamma_{CSF}}{\gamma_{APB}} = \frac{221 \text{ mJ/m}^2}{172 \text{ mJ/m}^2} = 1.28
\]

(23)

At the same time, according to a previous estimation of energy barrier in Ni-based superalloy [20] the ratio between barrier and APB energy is estimated. Using these ratios as additional constraints, all the parameters are determined and compiled in Table 3.

Figure 19. The composition dependence of GSF surface. The GSF surfaces are obtained by fitting an analytic expression with data points which are obtained for the Ni-based, Co-based and CoNi-based superalloys. The 3-fold rotational symmetry is revealed by the white triangular, and the mirror planes are plotted with the white dashed lines.
Table 3. The parameters of the GSF surfaces of the $\gamma'$ phases.

<table>
<thead>
<tr>
<th></th>
<th>$c_0$</th>
<th>$c_1$</th>
<th>$c_2$</th>
<th>$c_3$</th>
<th>$c_4$</th>
<th>$c_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni-based</td>
<td>978.9</td>
<td>-91.47</td>
<td>81.2</td>
<td>-240.2</td>
<td>-33.36</td>
<td>17.07</td>
</tr>
<tr>
<td>CoNi-based</td>
<td>412.4</td>
<td>-21.29</td>
<td>24.99</td>
<td>-97.93</td>
<td>-24.57</td>
<td>20.45</td>
</tr>
<tr>
<td>Co-based</td>
<td>660</td>
<td>-33.47</td>
<td>39.68</td>
<td>-156.6</td>
<td>-39.69</td>
<td>33.19</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>$c_6$</th>
<th>$c_7$</th>
<th>$c_8$</th>
<th>$c_9$</th>
<th>$c_{10}$</th>
<th>$c_{11}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni-based</td>
<td>-26.21</td>
<td>189.4</td>
<td>-426.6</td>
<td>44.57</td>
<td>-8.031</td>
<td>9.583</td>
</tr>
<tr>
<td>CoNi-based</td>
<td>-14.74</td>
<td>75.78</td>
<td>-179.6</td>
<td>16.26</td>
<td>-13.85</td>
<td>-0.5898</td>
</tr>
<tr>
<td>Co-based</td>
<td>-23.72</td>
<td>121.1</td>
<td>-287.4</td>
<td>25.94</td>
<td>-22.53</td>
<td>-1.104</td>
</tr>
</tbody>
</table>

By using these fitting parameters, GSF potential surfaces for each composition are drawn in Figure 19. Three-fold axis and mirror planes are indicated on these potential surfaces.

There are no abnormal local minima or maxima, which means that the fitting result satisfies the constraint of the crystalline structure of $\gamma'$ phase.

In this work, GSF potential surface in the matrix phase always follows that of FCC Ni.

Since stacking-fault energy in matrix is a trivial effect when compared with $\gamma'$ phase stacking-fault energy, it is still a good assumption to use matrix GSF surface of Ni-based superalloy in the simulations of CoNi- and Co-based superalloys. The analytic expression of GSF surface in matrix is:
\[ I_\gamma = c_0 + c_1 \times (\cos \times (2\pi(\eta_1 - \eta_2)) + \cos(2\pi(\eta_2 - \eta_3)) + \cos(2\pi(\eta_3 - \eta_1))) \\
+ c_2 \times (\cos(2\pi(2\eta_1 - \eta_2 - \eta_3)) + \cos(2\pi(2\eta_2 - \eta_3 - \eta_1)) \\
+ \cos(2\pi(2\eta_3 - \eta_1 - \eta_2))) \\
+ c_3 \times (\cos(4\pi(\eta_1 - \eta_2)) + \cos(4\pi(\eta_2 - \eta_3)) + \cos(4\pi(\eta_3 - \eta_1))) \\
+ c_4 \times (\cos(2\pi(3\eta_1 - \eta_2 - 2\eta_3)) + \cos(2\pi(3\eta_2 - 2\eta_3 - \eta_1)) \\
+ \cos(2\pi(3\eta_3 - \eta_1 - 2\eta_2)) + \cos(2\pi(3\eta_3 - \eta_1 - 2\eta_2))) \\
+ c_5 \times (\sin(2\pi(\eta_1 - \eta_2)) + \sin(2\pi(\eta_2 - \eta_3)) + \sin(2\pi(\eta_3 - \eta_1))) \\
+ c_6 \times (\sin(4\pi(\eta_1 - \eta_2)) + \sin(4\pi(\eta_2 - \eta_3)) + \sin(4\pi(\eta_3 - \eta_1))) \\
+ c_7 \times (\sin(2\pi(2\eta_1 - 3\eta_2 + 3\eta_3)) + \sin(2\pi(3\eta_1 - 2\eta_2 - \eta_3)) \\
+ \sin(2\pi(-2\eta_1 - \eta_2 + 3\eta_3)) + \sin(2\pi(\eta_1 + 2\eta_2 - 3\eta_3)) \\
+ \sin(2\pi(-3\eta_1 + \eta_2 + 2\eta_3)) + \sin(2\pi(-\eta_1 + 3\eta_2 - 2\eta_3))) \\
\]

(24)

The parameters are compiled in Table 4.

<table>
<thead>
<tr>
<th>\gamma matrix</th>
<th>(c_0)</th>
<th>(c_1)</th>
<th>(c_2)</th>
<th>(c_3)</th>
<th>(c_4)</th>
<th>(c_5)</th>
<th>(c_6)</th>
<th>(c_7)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\gamma) matrix</td>
<td>73.27</td>
<td>-20.25</td>
<td>-4.22</td>
<td>-0.22</td>
<td>0.14</td>
<td>-22.82</td>
<td>7.75</td>
<td>1.64</td>
</tr>
</tbody>
</table>

Table 4. The parameters of the GSF surfaces of the \(\gamma\) matrix.
2.6. Summary

(1) The generalized stacking-fault (GSF) potential energy landscape of the γ" phase has been determined by DFT calculations. Two unique, unstable stacking-faults (SFs), i.e., APB-like stacking fault and CSF, have been identified. After they are created during deformation, they transform spontaneously to the nearby stable SFs on the GSF energy surface and create additional dislocation contents.

(2) The ISF energy in γ" was determined to be extremely low (~2.3 mJ/m^2). However, the energy barrier of the deformation pathway along ISF was determined to be~252 mJ/m^2, which is close to that of the deformation pathway along ISF in the γ matrix. The extremely low energy and the moderate barrier suggest an abundance of ISF in γ" particles in IN718[3].

(3) The generalized stacking-fault (GSF) potential energy landscape of the γ’ phase was determined by fitting an analytical expression with experimental observations of APB energy and SISF energy. The composition dependence of the GSF’s surface was calculated for use as an input to the phase field simulations.
The physical parameters used in this chapter follow the values in the literature [82], except for the GSF surface of the $\gamma''$ phase, which was calculated using the DFT method.

3.1. **Phase-field simulation of dislocation shearing of $\gamma''$ precipitates**

In Figure 20, GSF surfaces of three variants of $\gamma''$ phase are plotted. The yellow and red arrows indicate Burgers vectors of full and partial dislocations respectively, and the green arrows show emitted partial dislocations which are created by unstable SF $\rightarrow$ stable SF transformations. For a given dislocation which originates from the matrix, e.g., AB in the Thompson notation, its interaction with each of the three variants of the $\gamma''$ phase will no longer be identical. For example, the AB dislocation will create an APB in Variant 2, while in Variant 1 and Variant 3 APB-like stacking fault unstable faults are formed. The unstable faults, once created, transform into a nearest stable configuration spontaneously. This process produces additional dislocation components. Thus, the strengthening mechanism of each variant must be considered separately.

Besides the AB matrix dislocation, an AC+AB matrix dislocation pair is also considered. Both of them are driven by an external applied stress of 800 MPa along the AC + AB direction. Looping or shearing process happens depends on details of the interactions.
Figure 20. The GSF potential energy surfaces for the three $\gamma''$ variants obtained from DFT calculation. Symbols which represent stacking faults are explained in the legend, and the corresponding Burgers vectors of the faults are shown in the inset.

In Figure 21, the interactions between a $1/2[1\bar{1}0]$ (AB) dislocation and the three different variants of $\gamma''$ particles are displayed. For each variant, the crystalline energy contours are drawn, with detailed dislocation and stacking fault configurations outlined in the bottom plots. The bottom plots is calculated by using the displacement field. In Figure 21, arrays of identical particles are used in the computational cells, which satisfies periodical boundary condition in the phase field simulations.
The dislocation is initiated at the deformation stage when particles have not been sheared. The deformation process is driven by a shear stress (800 MPa) on the (111) plane along the [-12-1] (i.e., Aδ or AC+AB), which causes the dislocation movement upwards. In Variant 1, δB leading partial is the only one that cuts through the particle and creates an ISF, while the Aδ trailing partial is blocked by the precipitate boundary. The Aδ loops around the particle, or its passing through will create a high energy APB-like SF which is unstable (as indicated in Figure 5). In Variant 2, the full dislocation loops around the particle, or its passing through will create a high energy APB in the particle. In Variant 3, the deformation pathway is δB + Aδ. This deformation results in an APB-like SF (see Figure 5) at the tip of the particle. This SF is unstable. Once it is created it transforms spontaneously to a nearby ISF (see the inset), which creates a δC loop (new dislocation content) at the boundary of ISF. The δC partial finally combines with the AB full dislocation in the γ″ phase and form a compact 1/3[121] super-dislocation. This super-dislocation cuts through the γ″ particle and leaves ISF as debris. It should be mentioned that in the crystalline energy contours shown in Figure 6 (and also in Figure 7 which will be discussed later), the ISF is almost indistinguishable from the perfect due to its ultra-low energy. When δC loop reaches the particle boundary, it will further pass through the γ matrix phase under the applied stress, since the energy of ISF in the γ phase is also low (~20mJ/m²).
Figure 21. The crystalline (stacking fault) energy contour displays the interaction between an AB dislocation and the three variants of $\gamma''$ particles. The top figures indicate the total energy contour and the bottom figures show schematically the corresponding dislocation and fault configurations in both $\gamma''$ and $\gamma'$ phases. The white arrow indicates the Burgers vector (AB) of the full dislocation and the red arrow indicates the applied stress direction.

To draw a conclusion, the deformation pathway of AB in the Varint 3 of $\gamma''$ phase is

$\delta B \rightarrow A\delta \rightarrow \delta C$ (see Figure 5). At the same time, the actual dislocation configuration that
determines the CRSS of AB shearing of Variant 3 is the creation of the 1/3[\overline{1}2\overline{1}] super-dislocation in the \(\gamma''\) particle that involves SF transition accompanied by the creation of a \(\delta C\) partial loop.

In Figure 22 and Figure 23, snapshots of the simulations are displayed which corresponds to AC+AB dislocation pair (i.e., a 1/2<112> type dislocation group) shearing process in each variant of \(\gamma''\) phase. Deformation processes in all three \(\gamma''\) variants are identified, which create different types of SF ribbons and final deformed microstructures. In both Variant 1 and Variant 2, SISF-ribbons are accompanied by a spontaneous transition from APB-like stacking fault to ISF at the tips of the particles. New dislocation components (\(\delta C\) in Variant 1 and \(\delta B\) in the Variant 2) are emitted. In Variant 3, AC dislocation tends to cut into the \(\gamma''\) particle and create an APB-like structure. This APB-like structure actually attracts the leading partial of following AB, i.e., \(\delta B\). As a result, the dislocation reaction converts the APB-like structure to a nearby ISF. At the same time, \(\delta B\) and AC dislocations team up and form a 1/3[\overline{1}2\overline{1}] super-dislocation inside \(\gamma''\) particle. For the trailing partial of the AB dislocation, i.e., A\(\delta\), it can easily cut into \(\gamma''\) particle and restores perfect crystal structure. As a result, inside \(\gamma''\) particle, an ISF-ribbon is created. It is bounded by a super-dislocation on the front side and the A\(\delta\) partial on the rear side. Besides the SF ribbons, dislocation nodes are also created in the case of Variant 1, which implies dislocation reaction and changing of partial dislocation sequence inside the \(\gamma''\) particle.
The detailed shearing pathways are shown on the GSF surface in Figure 20. In Variant 1, the AC+AB dislocation pair goes through the shearing pathway of \( \delta B \rightarrow A\delta \rightarrow \delta C \rightarrow A\delta \). This pathway is indicated by the red arrows in Figure 20. The dislocation sequence inside \( \gamma'' \) particle is changed from that in the matrix. Although the leading partial (\( \delta C \)) of the front full matrix dislocation AC reaches particle boundary firstly, it tends to loop around \( \gamma'' \) particle until the leading partial (\( \delta B \)) from the rear full matrix dislocation AB cuts the particle. The \( \delta B \) partial from AB is the first partial to enter the \( \gamma'' \) particle and the dislocation sequence is changed at this stage. Among all partials of AC+AB, \( \delta B \) it is the only one that directly creates an ISF (with ultra-low energy) by itself. This cutting is followed by the two partials of AC, i.e., A\( \delta \) and \( \delta C \), and an SISF is created (Frame 1). In the next stage, the trailing partial (A\( \delta \)) of AB arrives and creates an unstable APB-like SF inside the \( \gamma'' \) particle. The deformed microstructure at this moment (Frame 2) consists of an SISF-ribbon which is bounded by an ISF on the front side and an APB-like SF on the rear side. This unstable APB-like SF immediately transforms to a stable and ultra-low energy fault, ISF. This transformation is spontaneous and accompanied by the emission of an additional dislocation loop (\( \delta C \)) (a new dislocation content, see Frame 3). This leads to a compact stacking fault ribbon configuration, ISF ribbon -> SISF ribbon -> ISF ribbon, which eventually shears through the \( \gamma'' \) particle.
Figure 22. (Frame 1 and Frame 2) The crystalline (stacking fault) energy contour displays the interaction between AC+AB dislocation pair and of γ” particles (grey color). Figures in the first row indicate the total energy contour, and the figures in the remaining rows show dislocation/SF configurations at three successive instances. The white arrows indicate AB and AC Burgers vectors, and the red arrow displays the applied stress direction.
Figure 23. (Frame 3 and Frame 4) The crystalline (stacking fault) energy contour displays the interaction between AC+AB dislocation pair and of γ″ particles (grey color). Figures in the first row indicate the total energy contour, and the figures in the remaining rows show dislocation/SF configurations at three successive instances. The white arrows indicate AB and AC Burgers vectors, and the red arrow displays the applied stress direction.
To draw a conclusion, the actual shearing deformation pathway (or mechanism) within Variant 1 of γ” by the AC+AB dislocation pair is δB→Aδ→δC→Aδ→δC. On the GSF surface, this pathway is shown by the red arrows in Figure 20 and the total displacement is AC+AB+δC. A debris shearing loop of δC expands into the γ matrix and ISF are created in both in γ” particle and γ matrix after the deformation. The actual fault configuration that determines the CRSS of AC+AB shearing of Variant 1 is the creation of the SISF ribbon in the γ” particle. Also, note that the dissociation sequence of AC dislocation along this deformation pathway becomes Aδ + δC rather than δC + Aδ (the conventional dissociation sequence). The dislocation sequence is changed from that in γ the matrix.

In Variant 2, the deformation pathway δC→Aδ→δB→Aδ is followed by the AC+AB dislocation pair, which is indicated by the red arrows in Figure 20. The leading partial (δC) from AC is the first one to cut into the γ” particle. The cutting process creates an ISF which is highly preferred energetically. In the next stage, the other remaining partials follow. Similar to the deformation process discovered in Variant 1, the resulting SF created by the remaining three partials is an unstable APB-like SF. Spontaneously, this unstable SF transforms to a nearby ISF, which is accompanied by the emission of a δB partial loop. Again, a compact ribbon structure is created and is ISF ribbon -> SISF ribbon -> ISF ribbon (Frame 3.), similar to what is found in Variant 1.

To draw a conclusion, the actual deformation pathway in Variant 2 is δC→Aδ→δB→Aδ→δB, and the total displacement in the precipitate is AC+AB+δB.
The fault configuration that determines the CRSS of shearing is again the creation of SISF ribbon. After the AC+AB pair cuts through Variant 2, an expanding dislocation loop of δB is left in the γ matrix and an ISF is left in the γ" particle, which is also similar to what is found in Variant 1.

In Variant 3, the deformation path of the AC+AB dislocation pair follows δC→Aδ→δB→Aδ (Figure 20,). Since AC+AB is a translational vector in this variant, there is no stacking fault debris left within the particle after the passage of the dislocation pair.

During the deformation, the AC dislocation first creates an APB-like fault that transforms spontaneously into an ISF, which leads to the creation of an ISF ribbon consisting of $\frac{1}{3}<112>$ super-dislocation, ISF and $\frac{1}{6}<112>$ partial. The CRSS of shearing through Variant 3 by the AC+AB dislocation pair is determined by the creation of the $\frac{1}{3}<112>$ super-dislocation.

3.2. Dislocation core structure in the deformation process related to AC+AB

Compared with the chemical energy contour, the dislocation core structure describes how the dislocation reaction and dissociate happen in terms of the displacement field. The dislocation core structure profile is an important input to the fast-acting yield strength model, which will be discussed later. The core structure profiles are plotted in two ways: the disregistry vs. spatial coordinate, and the dislocation density vs. spatial coordinate. In the following figures, the disregistry of each grid point is calculated as the magnitude of displacement field on this grid point. The dislocation density is calculated as the derivative of the disregistry. In both plots, the x-axis represents the grid number, while
the grid size of this calculation does not reveal the real core size. Consequently, the calculated density could be different from the realistic density by a scaling constant. However, since our calculation is focused on the qualitative characterization of the core structure, this scaling difference does not change the conclusion.

In Figure 24 and Figure 25, the core structure of AB+AC dislocation in Variant 1 of \( \gamma'' \) phase is displayed in three successive frames of the dislocation evolution simulation.

Figure 24. The AC+AB dislocation core profile inside the Variant 1 of the \( \gamma'' \) particles (Frame 1). The ISF and SISF are displayed as the intermediate stacking fault ribbons.
In Figure 24, a deformation pathway of $\delta B \to ISF \to A\delta + \delta C \to SISF \to A\delta$ is revealed by the core structure profile, which is consistent with the chemical energy contours. An SISF ribbon is relatively narrow, and the corresponding local minimum is not obvious in the dislocation density plot. This is due to the limited resolution in our calculation. Higher resolution will definitely reveal the more detailed structure of the SISF ribbon.

Figure 25. The AC+AB dislocation core profile inside the Variant 1 of the $\gamma''$ particles (Frame 2). The ISF and SISF are displayed as the intermediate stacking fault ribbons. The APB-like stacking fault appears and will transform into an ISF in the next Frame.
In Figure 25, a deformation pathway of δB—>ISF—>Aδ+δC—>SISF—>Aδ—>APB-like stacking fault is revealed by the core structure profile, which is consistent with the chemical energy contours. An APB-like stacking fault is created as the intermediate state which will finally transform into a nearby ISF. Again, the SISF ribbon is not obvious in the dislocation density plot, which is due to the limited resolution in this calculation. A minor shoulder is shown on the right of ISF, which is related to an APB-like stacking fault close to the ISF. Although this APB-like stacking fault is unstable, the geometry of the GSF surface is flattened by this APB-like stacking fault, and the dislocation density is increased in the vicinity of the APB-like stacking fault.

In Figure 26, Figure 27 and Figure 28, the core structure of the AB+AC dislocation in the Variant 2 of the γ” phase is displayed in three successive frames of the simulation.
Figure 26. The AC+AB dislocation core profile inside the Variant 2 of the γ" particles (Frame 1). The ISF and SISF are displayed as the intermediate stacking fault ribbons. The APB-like stacking fault appears and will transform into an ISF later.

In Figure 26, a deformation pathway of δC->ISF->Aδ+δB->SISF->Aδ->APB-like stacking fault is revealed by the core structure profile. This profile can be directly compared with the chemical energy contours. An APB-like stacking fault is created as the intermediate state which will finally transform into a nearby ISF. Between Aδ+δB and Aδ, an SISF ribbon is created but relatively narrow. When a higher resolution is applied in simulation, a local minimum of SISF will be observed.
Figure 27. The AC+AB dislocation core profile inside the Variant 2 of the $\gamma''$ particles (Frame 2). The ISF and SISF are displayed as the intermediate stacking fault ribbons. The APB-like stacking fault appears and will transform into an ISF in the next Frame.
Figure 28. The AC+AB dislocation core profile inside the Variant 2 of the γ" particles (Frame 3). The ISF and SISF are displayed as the intermediate stacking fault ribbons. The ISF is the final debris inside the particle.

In Figure 27, a deformation pathway of δC->ISF->Aδ+δB->SISF->Aδ->APB-like stacking fault is revealed by the core structure profile. The profile reveals the characteristics of the shearing process which is consistent with the chemical contours. An APB-like stacking fault is created as the intermediate state which will finally transform into a nearby ISF. An SISF ribbon is created between Aδ+δB and Aδ. The corresponding
local minimum is not obvious due to the limited resolution in this calculation. A negative peak is shown between Aδ and APB-like stacking fault and indicates an APB-like stacking fault -> ISF transition inside the ABP-like zone of the deformed γ" particle.

Figure 29. The AC+AB dislocation core profile inside the Variant 3 of the γ" particles (Frame 1). The APB-like stacking fault will transform into an ISF in the next Frame.

In Figure 28, a deformation pathway of δC->ISF->Aδ+δB +Aδ->ISF is revealed by the core structure profile. The profile reveals characteristics of the shearing process which is
consistent with the chemical contours. An APB-like stacking fault disappears inside the particle and an ISF is left as the debris of the deformation. An SISF ribbon disappears in this frame, because of two possible reasons. The first reason is the low resolution. The second reason is that $A\delta + \delta B + A\delta$ coupling is strong and the SISF ribbon is compressed. In Figure 29 and Figure 30, the core structure of $AB + AC$ dislocation in the Variant 3 of the $\gamma''$ phase is displayed in three successive frames of the simulation.

Figure 30. The $AC + AB$ dislocation core profile inside the Variant 3 of the $\gamma''$ particles (Frame 2). The ISF is the intermediate ribbon during the shearing process.
In Figure 29, a deformation pathway of AC->APB-like stacking fault->δB in γ″ particle is revealed by the core structure profile. The profile shows the characteristics of the shearing process which is consistent with the chemical contours. An APB-like stacking fault appears inside the particle as an intermediate state at the tip of the particle. It will transform into a nearby stable ISF.

In Figure 30, a deformation pathway of AC+δB->ISF->Aδ in a γ″ particle is revealed by the core structure profile. The profile shows the characteristics of the shearing process which is consistent with the chemical contours. The APB-like stacking fault disappears and is transformed into an ISF. However, a minor shoulder is shown on the left of the ISF, which is due to the existence of an APB-like stacking fault in the vicinity of the ISF. The geometry of the GSF surface is flattened by an APB-like stacking fault which is unstable, and in the vicinity of this APB-like stacking fault, the dislocation density is increased and a shoulder appears in the density plot.

APB is absent in the AC+AB dislocation core structures in three variants of γ″ phase. Instead, an ISF and an SISF are observed at each deformation stage, while an APB-like stacking fault appears at the early stages of the particle shearing. Meanwhile, only an 1/6 <112> dislocation loop and an ISF are left in the deformed microstructure. This result is consistent with the recent TEM observations in the creep IN718 superalloy [30, 65, 66]. In the experiment, for example, no individual 1/2 <110> type dislocations were found in
the γ phase and no ABPs were found in the γ” phase, and only the <112> type dislocations were identified in the γ phase.

3. 3. Deformation of 718-type microstructure

In the previous part, although the ISF is left as the final configuration in the γ” precipitates, our simulations indicated that SISF and APB-like stacking fault SF ribbons were the critical configurations that determined the strength of the γ” shearing. This behavior is shown in Figure 22 and 23.

In this part, phase field simulations were conducted to determine the statistics of stacking-fault configurations in the deformed microstructure, which provide a direct explanation of the TEM observations. Before that, the “realistic” microstructure of 718-type superalloy was simulated, which is the input of the phase-field deformation package.

3.3.1. Microstructure simulation

In contrast to the alloys with only one precipitate, in the alloys with multi-components the temporal evolutions of the volume fraction and particle size are not necessary to be monotonous. For example, the composition of the 718-type superalloy decides that its crystalline microstructure has multiple phases including the γ’, γ” and δ phases. The complex interaction between the dislocation and the multiple precipitates in the realistic microstructure controls dominating dislocation configurations and hardening mechanisms. In order to provide a physics-based model of the deformation properties of the 718-type superalloy, it is crucial to understand the evolution of the multi-phase microstructure firstly.
According to the previous work by N. Zhou [82], the 718-type microstructure can be simulated using the phase-field method based on the Kim-Kim-Suzuki treatment [83]. In his simulation, the aging process was accompanied by the co-precipitation of several phases (γ', γ'' and δ) from a the supersaturated matrix phase (γ). In my work, since the δ phase degrades the yield strength and can be avoided by suitable heat treatment, only the γ' and γ'' precipitates are considered.

The phase-field precipitate model uses the inputs including the Ni-Nb-Al pseudo-ternary thermodynamic database, lattice parameter, misfit strain of each precipitate phase, elastic modulus, the interfacial energy of the precipitate phases and the inter-diffusivities [82]. The Ni-Nb-Al pseudo-ternary thermodynamic database tells the precipitate volume fraction and the average particle size under the given processing condition. Using this database as an input, the phase-field simulation is able to reveal the particle spatial distribution and the particle size distribution.

PANDAT [84] software provides both the equilibrium and dynamic information of microstructure. In the equilibrium dataset, the equilibrium volume fraction and the stability of precipitate are revealed. However, in many cases, an alloy is not necessary to be heat treated for an extremely long time period which reaches thermodynamic equilibrium. In order to implement a model to predict the mechanical properties obtained through a realistic heat treatment condition, it is critical to use a dynamic dataset which predicts the volume fraction and average particle size of alloys which are used in the engine components. In Figure 31 and Figure 32, the evolution of the average particle size
and the volume fraction are predicted by using PANDAT software. The phase field simulation is applied to simulate the microstructure which has been heat-treated for $10^3$ mins.

![Graph showing dynamic evolution of volume fraction](image1)

**Figure 31.** The thermodynamic prediction of the dynamic evolution of the volume fraction in the 718-type superalloy.

![Graph showing dynamic evolution of particle size](image2)

**Figure 32.** The thermodynamic prediction of the dynamic evolution of the particle size in the 718-type superalloy.
According to the prediction by PANDAT software, at the beginning of the heat treatment, the $\gamma'$ phase is dominating while the volume fraction of the $\gamma''$ is only $1/3$ of that of the $\gamma'$ phase. In the later stage of the aging process, the $\gamma''$ phase volume fraction increases dramatically, while the $\gamma'$ phase volume fraction drops to $1/3$ of its original value. It should be mentioned that the $\gamma''$ phase is not a stable state but a metastable one.

Figure 33. The phase-field simulation of the microstructural evolution. Random particle nuclei are initiated in the Frame 1. The growth and the coarsening happen in the Frames 2, 3 and 4.
The alloy processing method has to be carefully controlled, otherwise, the $\gamma''$ phase could be consumed by the formation of the $\delta$ phase. As has been investigated by many other works, the mechanical properties of the superalloy will degenerate when the $\delta$ phase consumes the $\gamma''$ phase. In our study, the $\delta$ phase volume fraction is supposed to be a constant and to be concentrated at the grain boundaries, and the $\gamma''$ phase survivals after a long-term aging.

By using the aging results of the volume fraction and particle size which are predicted by PANDAT software, the phase-field simulation of the 718-type microstructure is performed. The volume fraction from PANDAT software decides the initial saturated composition in the $\gamma$ phase matrix. Meanwhile, the particle size from PANDAT software decides the termination condition of the phase field simulation. The simulation is initiated with the randomized nucleation. The particle growth and coarsening are governed by the time-dependent Ginzburg-Landau equation. In Figure 33, the microstructures at 4 frames are displayed. The simulation shows how the particle morphology, the size distribution, and the spatial distribution are established. These results are hard to be obtained through the current thermodynamics database. What is more, the phase-field simulation is able to simulate the particle morphology by considering the the elastic modulus and the misfit strain. Meanwhile, the particle size distribution and the spatial distribution are introduced by the randomness of the initial nuclei position.
In Figure 34, the spatial distribution of the precipitate is characterized by the channels between the γ" particles. The local channel width decides whether a dislocation line can loop around a particle or not. If a particle is connected with the narrow channels and the particle size is small, this particle tends to be sheared. On the other hand, if a large particle is connected with the wide channels, the Orowan looping is energetically preferred. The γ’ particles are ignored when calculating the the channel width since all the γ’ particles are assumed to be sheared during the deformation. This assumption is straightforward according to the TEM observations in which there is no Orowan looping around the γ’ particles.

Figure 34. The channel map and the particle spatial distribution in the 718-type microstructure. The γ” particles are displayed in the red color. The cyan-blue lines indicate the channels. The γ’ particles are assumed to be sheared.
The channel width distribution is shown in Figure 35, where a large variance is revealed. A combination of the shearing and the looping is expected, which needs to be calculated by the phase-field deformation simulations.

![Normalized histogram of channel width distribution](image)

**Figure 35.** The normalized histogram of the channel width distribution in the 718-type microstructure.

In Figure 36, the local CRSS to the Orowan looping is calculated based on the channel map of the 718-type superalloy, which determines the degree of the work hardening when dislocation sources are intensively distributed throughout the crystal. On the other hand, when the dislocation sources are rare in the crystal or largely concentrated at the grain boundaries, the CRSS to the Orowan looping is controlled by the closed zones bounded by the narrow channels in the vicinity of the dislocation source. The later scenario will be discussed in Chapter 5 of the fast-acting deformation model.
Figure 36. The CRSS map of the local Orowan looping strengthening in the 718-type microstructure. The $\gamma''$ particles are displayed as the white objects. The value in each triangular patch represents the Orowan looping strengthening to any dislocation loop originated inside the triangular patch. The strengthening (CRSS) is calculated by using the average channel width of triangular patches.

Figure 37. The channel width distribution when both the $\gamma'$ and $\gamma''$ particles are assumed to be looped.
Figure 38. The normalized histogram of the channel widths distribution in the 718-type microstructure is displayed when both the $\gamma'$ and $\gamma''$ particles are assumed to be looped.

Figure 39. The CRSS map of the local Orowan looping strengthening in the 718-type microstructure. Both the $\gamma''$ and $\gamma'$ particles are assumed to be looped. The value in each triangular patch represents the Orowan looping strengthening to any dislocation loop originated inside the triangular patch. The strengthening (CRSS) is calculated by using the average channel width of the triangular patch.
At the lower applied stress level, all particles (both $\gamma''$ and $\gamma'$) are assumed to be looped, and much narrower effective channels are expected. The channel-width-distribution peak shifts to <25nm according to Figure 38. As a result, the degree of the local work hardening is largely increased, which is indicated by more yellow colored patches in Figure 39. Again, this contour is meaningful only when the dislocation sources are intensively distributed throughout the crystal. The CRSS map in Figure 39 can be applied as an input to the creep rate model where the applied stress is low or the stacking-fault energy is high enough to prevent any particle shearing. It should be mentioned that, in most commercialized superalloys such as IN718, the stacking-fault energy of $\gamma'$ is relatively low. Consequently, there is very low correlation between work hardening and $\gamma'$ particles and only Figure 36 should be used as the input of the creep rate model.

3.3.2. **Behavior of emitted partial dislocation**

Due to the features of multiple phases / variants, any dislocation line is simultaneously associated with several different shearing mechanisms. This is also true for the partial dislocations created by the stacking fault transformation. Before any statistical investigation of the deformation process in the 718-type microstructure, several scenarios of the interaction between the emitted partial dislocation and the particles are simulated in this part. These simulation results provide one explanation of the $<112>$ type dislocation group observed by the TEM [30, 65, 66], assuming that the observed dislocation lines are those with the extremely low activity.
**1/6<112> type emitted dislocation pinned by γ' particle**

![Diagram of dislocation and γ' particle interaction](image)

Figure 40. The phase-field simulation of the interaction between the δC emitted dislocation with the γ' particle. The pinning effect is represented by the creation of the CSF inside the γ' phase. The entire crystal has already been sheared by the BA full dislocation. The GSF energy of the γ' phase is not scaled.

In Figure 40 and Figure 41, a partial dislocation created from the Variant 1 of the γ” phase is pinned by a nearby γ' phase particle. The pinning effect is due to the high energetic CSF energy in the γ' phase, as is shown in Figure 40. The dislocation movement can be either Orowan looping or particle shearing depending on the CSF.
energy of the $\gamma'$ phase, the particle size and the loading condition. The particle shearing happens when applied stress along the created partial is high, or when the particle size is small enough, or when the temperature is high (the CSF energy is significantly reduced). In Figure 41, the Orowan looping happens, since the applied stress is not sufficiently high to create a CSF inside the $\gamma'$ phase.

![Figure 41](image_url)

Figure 41. The phase-field simulation of the interaction between the $\delta C$ emitted dislocation and the $\gamma'$ particle. The pinning effect is represented by the Orowan looping around the $\gamma'$ particle. The entire crystal has already been sheared by the BA full dislocation. The GSF energy of the $\gamma'$ phase is scaled by a factor of 2.
1/6<112> type emitted dislocation pinned by γ" particle

In Figure 42, a partial dislocation created from the Variant 1 of the γ" phase is pinned by a nearby Variant 3 particle of the γ" phase. The pinning effect is due to the unstable and high-energetic CSF in the γ" phase. The dislocation movement can be either Orowan looping or particle shearing. Particle shearing is hard to happen in this scenario, since the applied stress level is not sufficiently high.

Figure 42. The phase-field simulation of the interaction between the δC emitted dislocation and the γ" particle. The pinning effect is represented by the Orowan looping around the γ" particle. The entire crystal has already been sheared by the AC+AB dislocation group.
**δC+δB type dislocation group related to AB+AC**

In Figure 43, two partial dislocations (δC and δB) are created from the Variant 1 and the Variant 2 of the γ" phase, respectively. They together form a 1/6<112> type dislocation group which is immobile in the γ matrix. These two dislocation loops both tend to expand but finally pin each other since the resolved shear stresses on these loops are equal in the magnitude. According to the GSF surface of the γ phase, the δC and δB dislocations cannot interact in the matrix, or a maximum stacking-fault energy would be created. The only way to move this dislocation group is to apply a shear stress which resolves different magnitude on these two Burgers vectors. In this scenario, the dislocation group will continuous to move until it reaches a γ/γ" boundary. When the applied stress magnitude is relatively low, this δC+δB dislocation group will be immobile again at the γ/γ" boundary, since δB and δC cannot interact inside the γ" phase.

However, when applied stress magnitude is high enough, the δC+δB group will be pushed into the γ" particle, and a CSF will be created. Since the CSF is unstable, it will transform spontaneously into a nearby restored crystalline structure. This transformation is accompanied by a creation of the Aδ type dislocation loop which is able to expand throughout the matrix.

Depending on the direction of the applied stress, two scenarios of the γ" particle shearing are displayed by the phase-field simulations. The particle shearing is caused by δC+δB
type dislocation group movement. In Figure 44 and Figure 45, shearing of the Variant 1 is displayed. In Figure 46 and Figure 47, shearing of the Variant 2 is shown. In both variants, the $A\delta$ dislocation loop is created and expands throughout the matrix. In the final deformed configuration, the $A\delta$ dislocation loops around one of the $\gamma''$ particles and a debris of $1/6<112>$ dislocation is left.

Figure 43. The phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which is immobile inside the $\gamma$ matrix. The pinning effect is due to the prohibited dislocation reaction. The entire crystal has already been sheared by the $AC+AB$ dislocation group.
Figure 44. The early four frames of the phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which moves through the $\gamma''$ particle under the applied stress along the $\delta B$ direction. The $A\delta$ loop is emitted when the $\delta C+\delta B$ dislocation group cuts though the Variant 1 particle of the $\gamma''$ phase. The $A\delta$ loop is later pinned by the Variant 2 particle of the $\gamma''$ phase. The entire crystal has already been sheared by the $AC+AB$ dislocation group.
Figure 45. The last four frames of the phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which moves through the $\gamma''$ particle under the applied stress along the $\delta B$ direction. The $A\delta$ loop is pinned by the Variant 2 particle of the $\gamma''$ phase. The only stacking fault debris is the ISF in the Variant 2 particle of the $\gamma''$ phase. The entire crystal has already been sheared by the $AC+AB$ dislocation group.
Figure 46. The early four frames of the phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which moves through the $\gamma''$ particle under the applied stress along the $\delta C$ direction. The $A\delta$ loop is emitted when the $\delta C+\delta B$ dislocation group cuts though the Variant 2 particle of the $\gamma''$ phase. The $A\delta$ loop is later pinned by the Variant 1 particle of the $\gamma''$ phase. The entire crystal has already been sheared by the $AC+AB$ dislocation group.
Figure 47. The last two frames of the phase-field simulation of the $\delta C+\delta B$ emitted dislocation group which moves through the $\gamma''$ particle under the applied stress along the $\delta C$ direction. The $A\delta$ loop is pinned by the Variant particle of the $\gamma''$ phase. The only stacking fault debris is the ISF in the Variant 1 particle of the $\gamma''$ phase. The entire crystal has already been sheared by the AC+AB dislocation group.

**<112> type immobile dislocation group created by AB pair on the Variant 1 $\gamma/\gamma''$ boundary**

In Figure 48 and Figure 49, when an AB pair dislocation deforms a crystal containing only the Variant 1 of the $\gamma''$ particle, an immobile dislocation group can be formed at the $\gamma/\gamma''$ boundary following the particle shearing. Actually, these two partial dislocations ($A\delta$ and $C\delta$) cannot interact with each other in the $\gamma$ matrix or the $\gamma''$ particle. A maximum stacking-fault energy would be created if the interaction happens in the $\gamma$ matrix, which is almost impossible. Also, the dislocation group cannot cut into a $\gamma''$ particle, or an unstable and high-energetic CSF would be created. The only way to move this dislocation group is to apply a shear stress which resolves a higher magnitude on the $C\delta$. Then the $A\delta+C\delta$ group can move through the matrix.
Figure 48. The early four frames of the phase-field simulation of the AB pair cutting through the Variant 1 particle of the $\gamma''$ phase. The $A\delta+C\delta$ dislocation group is created which is impossible to move since the $A\delta$ and $C\delta$ cannot interact.
Figure 49. The last two frames of the phase-field simulation of the AB pair cutting through the Variant 1 particle of the $\gamma''$ phase. The A$\delta$+C$\delta$ dislocation group is created which is impossible to move since the A$\delta$ and C$\delta$ cannot interact.

In this simulation, the perfect stacking sequence is restored inside the $\gamma''$ particle. At the same time, a debris of the $1/6<112>$ type dislocation group is left on the particle boundary. The movement of the trailing AB dislocation will be reduced since its partial A$\delta$ is involved in this looping process. In the microstructure of Figure 49 where the inter-particle distance is much larger than the particle size, the reduction of the deformation rate is not obvious. However, in a realistic microstructure where the inter-particle distance is comparable or even smaller than the average particle size, the Orowan looping strength will be significant and the movement rate of the trailing AB will be largely reduced. As a result, a decoupling between the leading and the trailing AB will be observed in a realistic 718-type microstructure. What is more, the immobile A$\delta$+C$\delta$ group eventually increases the CRSS of the trailing AB movement, which causes less activity of the AB pair. As a result, the AB pair dislocation group will hard to be
observed inside the deformed microstructure when the dislocation sources are rare in the crystal or largely concentrated at the grain boundaries.

*<112> type immobile dislocation group created by AB pair on the Variant 3 $\gamma''/\gamma$ boundary*

In Figure 50 and Figure 51, when the AB pair dislocation deforms a crystal containing only the Variant 3 of the $\gamma''$ particle, an immobile dislocation group can be formed at the $\gamma'/\gamma''$ boundary after the particle shearing. Actually, the two partial dislocations at the boundary ($\delta B$ and $\delta C$) cannot interact with each other in the $\gamma$ matrix or the $\gamma''$ particle. If the reaction happens in the $\gamma$ matrix, a maximum stacking-fault energy would be created. Inside the $\gamma''$ particle, the creation of an unstable and high-energy CSF is hard. Again, The only way to move this dislocation group is to apply a shear stress which resolves a higher magnitude on the $\delta C$. Then the $\delta B+\delta C$ group can move through the matrix.
Figure 50. The early four frames of the phase-field simulation of the AB pair cutting through the Variant 3 particle of the $\gamma^\prime\prime$ phase. The $\delta B + \delta C$ dislocation group is created which is impossible to move since the $\delta B$ and $\delta C$ cannot interact.

In the deformed microstructure, the perfect stacking sequence is restored inside the Variant 3 of the $\gamma^\prime\prime$ particle. Meanwhile, the $1/6<112>$ type dislocation group is left as a debris on the $\gamma/\gamma^\prime\prime$ boundary. Since its partial $\delta B$ is involved in the looping process of the later stage of the deformation, the moving rate of the trailing AB dislocation will be reduced. The reduction of the deformation rate is trivial in Figure 50 since in the microstructure the inter-particle distance is much larger than the particle size. However, in a microstructure of a realistic 718-type superalloy, where the inter-particle distance is
comparable or even smaller than the average particle size, the looping effect can significantly reduce the moving rate of the trailing AB. As a result, a decoupling between the leading and the trailing AB is expected. The immobile $A\delta + C\delta$ group eventually causes less activity of the AB pair dislocation group, and the CRSS of the trailing AB movement is increased. As a result, inside the deformed microstructure where the dislocation sources are rare in the crystal or largely concentrated at the grain boundaries, the population of the AB pair should be small.

Figure 51. The last four frames of the phase-field simulation of the AB pair cutting through the Variant 3 particle of the $\gamma''$ phase. The $\delta B + \delta C$ dislocation group is created which is impossible to move since the $\delta B$ and $\delta C$ cannot interact.
3.3.3. **Phase-field simulation of deformation in realistic 718-type microstructure**

In order to investigate the dominating deformation mechanisms in the 718-type superalloys, the phase-field simulations are performed in a realistic precipitate microstructure. The microstructure represents the spatial and size distributions of the $\gamma'$ and the $\gamma''$ particles. The ab initio GSF surface is applied to describe the stacking fault inside particles, as has been discussed in chapter 2.

Several different dislocation configurations are initiated to interact with the precipitate microstructure. The crystalline energy contours are displayed in Figure 52, Figure 53, Figure 54, Figure 55, Figure 56 and Figure 57. These simulations are performed at 500 MPa, and the applied stress direction is along the Burgers vector of each dislocation group.

**$\frac{1}{2}\langle110\rangle$ single dislocation**

When the magnitude of the applied stress is only 500 MPa, AB single dislocation is very hard to move through the 718-type microstructure. As is shown in Figure 52, after the shearing of the $\gamma'$ particles in the vicinity of the initial dislocation location, the dislocation is stopped by the $\gamma''$ particles. A Variant 2 $\gamma''$ particle is looped in this simulation since the surrounding channels are relatively wide. Around this looped $\gamma''$ particle, there are only $\gamma'$ particles which provide a weak friction force to the Orowan looping. The sheared $\gamma'$ particles are displayed in the green and yellow colors which correspond to the APB and the CSF respectively. Inside the channels between the $\gamma''$ particles, there is no significant
de-correlation between the leading and trailing partials, due to the existence of the $\gamma'$ phase which prevents the dissociation of the AB dislocation. The dissociation would cause the formation of a CSF inside the $\gamma'$ particles, which is energetically unfavorable.

Figure 52. A deformation process is simulated by the phase-field method when an AC single dislocation interacts with a 718-type microstructure. The AC dislocation is unable to percolate through the microstructure, due to the strong pinning effect from the $\gamma''$ phase.

$\frac{1}{2}<110>$ pair dislocation group

When an AC pair interacts with the Variant 1 of the $\gamma''$ particle in Figure 53 and Figure 54, the Orowan looping happens. As is shown in the deformation pathways, in contrast to the classic understanding, the spontaneous stacking fault transition changes the
deformation pathway of the AC pair from reaching APB in the Variant 2 and the Variant 3 of the $\gamma''$ phases. An $1/6<112>$-type dislocation group is formed by the two partial dislocations. These two partials cannot react nor cut into the $\gamma''$ particles. In the Variant 2, $B\delta + A\delta$ creates the $\delta C$-type dislocation group, and in the Variant 3 the $\delta B + \delta C$ forms the $A\delta$-type dislocation group.

Figure 53. The early stages of a deformation process are simulated by the phase-field method when an AC pair interacts with a 718-type microstructure. The dislocation loops are left at the $\gamma/\gamma''$ boundaries while the $\gamma'$ particles are sheared.

Due to the immobility of these $1/6<112>$ type dislocation groups, the trail partial of the second AC (which processes one component of the $1/6<112>$-type dislocation group) has
to loop around a particle. At the same time, the first AC and the leading of the second AC can easily move through the $\gamma''$ particles by creating the APB-like stacking fault ribbon. Another feature of the AC pair shearing is that the dislocation coupling follows different rules inside and outside the $\gamma''$ particle. Inside the $\gamma''$ particles, the first AC and the leading partial of the second AC tend to move together, while the trailing partial of the second AC is left behind. At the same time, in the matrix, there is no such a coupling between the first AC and the leading partial of the second AC.

Consequently, the movement of the second AC slows down. Indeed, the deformation rate of the second AC’s trailing partial is largely reduced by the $\gamma/\gamma''$ boundary, since the second AC’s trailing is one component of the immobile dislocation group. At the same time, according to the GSF surface, the dissociation in the matrix is not preferred by the applied stress. As a result, the slower trailing dislocation drags the leading dislocation by the force of stacking-fault energy, and the leading partial’s movement also slows down.

To draw a conclusion, the deformation rate of the second AC is controlled by its trailing, and this AC is significantly decoupled from the first AC.

When the average particle size is small and the inter-particle spacing is narrow, the decoupling effect by the Variant 2 and the Variant 3 will be significant and the CRSS of AC will be increased. At the same time, the Orowan looping around the Variant 1 contributes a larger strengthening effect when the channel width is narrower. As a result, in a $\gamma''$ dominating superalloy such as IN718, AC pair will be hard to be activated. That is
one of the reasons why the $<110>$-type dislocation is not observed in the deformed IN718 alloy.

Figure 54. The later stages of a deformation process are simulated by the phase-field method when an AC pair interacts with the 718-type microstructure. The dislocation loops are left at the $\gamma/\gamma''$ boundaries while the $\gamma'$ particles are sheared. The leading and trailing ACs are decoupled, which implies a slower deformation rate of the trailing AC.

$\frac{1}{2}<110>$ quadruplet dislocation group

The deformation by the AC quadruplet is more complex at the first glance. Similar with the deformation by the AC pair, in contrast to the classic understanding, the spontaneous stacking fault transition changes the deformation pathway of the AC quadruplet from reaching the perfect crystal structure in the Variant 2 and the Variant 3 of the $\gamma''$ phase.
Figure 55. The early stages of a deformation process are simulated by the phase-field method when an AC quadruplet interacts with a 718-type microstructure. The components of this quadruplet are decoupled, which implies a slower deformation rate.
Figure 56. The later stages of a deformation process are simulated by the phase-field method when an AC quadruplet interacts with a 718-type microstructure. The components of this quadruplet are decoupled, which implies a slower deformation rate. The trailing two ACs are stopped in the vicinity of their initial location.

Similar to the AC pair, a 1/3<112> type dislocation group is formed which cannot cut into the γ" particle. In the Variant 3, two Bδ together with two Aδ creates two δC-type dislocation group. Similar with the δC dislocation group in the AC pair case, these two δC cannot cuts into the Variant 3 of the γ" particle, or a maximum energy would be reached. Due to the formation of this 1/3<112> type dislocation group, the trail partials of the third and the fourth ACs (which are the components of this dislocation group) have to loop around the γ" particles. At the same time, the first two ACs and the leading partials of the third and the fourth ACs can easily move through the γ" particles by forming multiple APB-like stacking fault ribbons. As a result, in the γ" particles, the first two ACs and the leading partials of the last two ACs tend to move together, while the trailing
partials of the last two ACs are left behind. At the same time, in the \( \gamma \) matrix, there is no such coupling between full dislocation and the partials of other full dislocations. Consequently, movement of the third and the fourth ACs slows down. Indeed, the deformation rate of the third and the fourth AC’s trailing partials is largely reduced by the \( \gamma/\gamma'' \) boundary, since the third and the fourth AC’s trailing partials are a component of the immobile dislocation group. At the same time, according to the GSF surface, the dissociation in the matrix is not preferred by the applied stress. As a result, the slower trailing dislocations drags the leading partials by the force of the stacking-fault energy, and the leading partials’ movement also slows down. To draw a conclusion, the deformation rate of the third and the fourth AC is controlled by their trailing partials, and these ACs are significantly decoupled from the first and the second ACs.

In the Variant 2, the AC quadruplet shearing happens and the perfect crystal structure is restored. But the deformation pathway does not follow the classic prediction. The additional B\( \delta \) partials are created due to the stacking fault transformation. The perfect crystal structure is reached when these B\( \delta \) partials are pushed back into the particle by following two A\( \delta s \)' shearing. This structure restoration is accomplished through the ABP-like ribbon and the SISF ribbon, instead of the APB ribbons.

Similar to the reasons of high CRSS of the AC pair, in a \( \gamma'' \) dominating superalloy, such as IN718, AC quadruplet is hard to be active. That is one of the reasons why the \(<110>\)-type dislocation group is not observed in the deformed 718-type superalloy.
\( 1/2<112> \) \((\text{AC+AB})\) dislocation group

In contrast to the AC pair or the AC quadruplet whose trailing partials have to loop around the \( \gamma'' \) particles due to the stacking fault transformation, the AC+AB dislocation group movement is actually enhanced by the spontaneous stacking fault transition. As is shown in Figure 57, during the particle shearing, the AC+AB will create stacking fault ribbons in all the variants of the \( \gamma'' \) phase. In the Variant 1 and the Variant 2 of the \( \gamma'' \) phase, an SISF ribbon and an ABP-like with very high energy are created firstly. The following spontaneous stacking fault transition removes the APB-like stacking fault and leaves an ISF whose stacking-fault energy is only \(~2 \text{ mJ/m}^2\). In the Variant 3, the AC overcomes the GSF barrier, creates an APB-like stacking fault as an intermediate state. Then the APB-like structure spontaneously transforms into an ISF whose energy is ultra-low. Finally, the trailing partial B\( \delta \) of the AB restores the perfect crystal of the \( \gamma'' \) phase.

To draw a conclusion, the deformation by the AC+AB only creates the stacking fault ribbons which are narrow and easy to move.

What is more, the AC and the AB are strongly coupled, since the dislocation reaction between the AC and the AB is required to form a stacking fault ribbons. In the Variant 1, the AC can only move after the leading of AB (\( \delta \text{B} \)) which creates the ISF. In the Variant 2, the AC and the the leading of the AB together create the stable SISF. In the Variant 3, the AC and the leading of the AB (\( \delta \text{B} \)) together create the ISF. The coupling AC+AB is consistent with the TEM observation where only \(<112>\)-type dislocation group is observed while any individual \(<110>\)-type dislocation is absent.
Figure 57. A deformation process is simulated by the phase-field method when an AC+AB group interacts with a 718-type microstructure. The components of this group are strongly coupled, which implies a relatively high deformation rate. Only the $\frac{1}{2}<11\bar{6}>$ type dislocation loops are left at the $\gamma'/\gamma''$ boundaries as the debris. The $\gamma'$ particles are sheared and an APB area is created.

However, besides the AC+AB’s easy shearing through the $\gamma''$ particles, the AC+AB is significantly pinned by the $\gamma'$ particles. Actually, the AC+AB creates APB in the $\gamma'$ phase which has very high energy. In the 718-type superalloy, this pinning effect is minor, since the $\gamma'$ phase has relatively lower volume fraction.
To draw a conclusion, the activation of the AB+AC dislocation group is easier than that of the AC pair when the particle size is still small (15-30 nm), since the percolation of the AB+AC does not produce any high energetic stacking fault debris in the $\gamma''$ phase, or is accompanied by any decoupling process. Although the AB+AC creates the APB in the $\gamma'$ phase, in most commercial 718-type alloys the existence of the $\gamma'$ phase is far rare compared with the $\gamma''$ phase and the AB+AC should be the dominating deformation mechanism in these alloys. Our simulation results of the AC quadruplet deformation display similar phenomena as the deformation by the AC pair. For the AC quadruplet, the $<112>$ type immobile dislocation group is formed. At 500 MPa, only the first two AC can shear through the crystal while the following two ACs are totally stopped due to the significant existence of the immobile dislocation groups.

It should be mentioned that the $<112>$-type dislocation debris exists in each scenario (the AC single dislocation, the AC dislocation pair, the AC dislocation quadruplet, or the AC+AB group). As a result, even when the AC pair or the AC quadruplet dislocation group is active, the $<112>$-type dislocation should also be observed in a large amount.

3.3.4. **Stacking fault population of deformed 718-type microstructure**

The stacking fault configurations in the deformed alloy reveals information of the deformation process and the competition among different energy terms. Also, the stacking fault debris is always related with other deformation phenomena such as twin formation and segregation. In this part, the statistics on the stacking fault population are calculated for each scenario.
½<110> pair dislocation group

The dominating stacking fault configurations in the Variant 1 (Figure 58), the Variant 2 (Figure 59) and the Variant 3 (Figure 60) of the γ” particles are the perfect stacking sequence, the ISF, and the perfect stacking sequence, respectively. In the γ’ (Figure 61) and the γ (Figure 62) phases, the perfect stacking sequence is the dominating structure, which is a result of the structural restoration by the AC pair in the simple cubic structure and the FCC structure.

Figure 58. The stacking fault configuration distribution in the Variant 1 of the γ” phase. The original structure is dominating, which implies that the Orowan looping happens on the γ/γ” boundaries of the Variant 1.
Figure 59. The stacking fault configuration distribution in the Variant 2 of the $\gamma''$ phase. The ISF is dominating, which implies that the stacking fault transformation happens in most Variant 2 $\gamma''$ particles. Meanwhile, the restored structure corresponds to the stacking fault transformation from the CSF to the perfect stacking sequence. Very little APB area is observed, which means the traditional AC pair shearing models, which predicts a large amount of APB, indeed fail.

Figure 60. The stacking fault configuration distribution in the Variant 3 of the $\gamma''$ phase. The restored structure is dominating, which implies the stacking fault transformation from the CSF to the perfect stacking sequence. Again, very little APB area is observed, which means the traditional AC pair shearing models indeed fail.
Figure 61. Stacking fault configuration distribution in the $\gamma'$ particles. The restored structure is dominating, which is consistent with the Burgers vector of AC pair.

Figure 62. The stacking fault configuration distribution in the $\gamma$ matrix. The restored structure is dominating, which is consistent with the Burgers vector of the AC pair.

$\frac{1}{2}<110>$ quadruplet dislocation group

The dominating stacking fault configurations in the Variant 1 (Figure 63), the Variant 2 (Figure 64) and the Variant 3 (Figure 65) of the $\gamma''$ particles are the perfect stacking
sequence, the ISF, and the perfect stacking sequence, respectively. Again, in the $\gamma'$ (Figure 66) and the $\gamma$ (Figure 67) phases, the perfect stacking sequence is the dominating structure, which is a result of the structural restoration by the AC quadruplet in the simple cubic structure and the FCC structure.

Figure 63. The stacking fault configuration distribution in the Variant 1 of the $\gamma''$ phase. The original structure is dominating, which implies that the Orowan looping happens on the $\gamma'/\gamma''$ boundaries of the Variant 1.
Figure 64. The stacking fault configuration distribution in the Variant 2 of \(\gamma''\) phase. The ISF is dominating, which implies that stacking fault transformation happens in most Variant 2 of the \(\gamma''\) particles. Meanwhile, the restored structure corresponds to the stacking fault transformation from the CSF to the perfect stacking sequence. Very little area of the restored structure is observed, which means the traditional AC quadruplet shearing models, which predicts a large amount of the restored structure, indeed fail.

Figure 65. The stacking fault configuration distribution in the Variant 3 of the \(\gamma''\) phase. The restored structure is dominating, which implies the stacking fault transformation from the CSF to the perfect stacking sequence. Again, very little area of the restored structure is observed, which means the traditional AC quadruplet shearing models indeed fail.
In Figure 67, which displays the stacking fault population in the γ matrix deformed by the AC quadruplet, there is no obvious peak observed between the third and the fourth
“restored” peaks. Although an ISF peak is expect between them, since half of the crystal has not been sheared by the trailing two AC dislocations, this ISF is not actually formed. The trailing two AC dislocations are stopped at the vicinity of the dislocation source.

1/2<112> (AC+AB) dislocation group

The dominating stacking fault configurations in the Variant 1 (Figure 68), the Variant 2 (Figure 69) and the Variant 3 (Figure 70) of the γ” particles are the ISF, the ISF, and the perfect stacking sequence, respectively. In the γ’ (Figure 71) phases, the APB is the dominating structure. In the the γ (Figure 72) matrix, the perfect stacking sequence is the major configuration. These configurations of the γ’ particles and the γ matrix are consistent with the Burgers vector of the AC+AB.

Figure 68. The stacking fault configuration distribution in the Variant 1 of the γ” phase. The ISF is dominating, which implies the stacking fault transformation from the APB-like stacking fault to the ISF.
Figure 69. The stacking fault configuration distribution in the Variant 2 of the $\gamma''$ phase. Again, the ISF is dominating, which implies the stacking fault transformation from the APB-like stacking fault to the ISF.

Figure 70. The stacking fault configuration distribution in the Variant 3 of the $\gamma''$ phase. The restored structure is expected to be created the Burgers vector of the AC+AB.
Figure 71. The stacking fault configuration distribution in the $\gamma'$ particles. The APB is dominating, which is consistent with the Burgers vector of the AC+AB.

Figure 72. The stacking fault configuration distribution in the $\gamma$ matrix. The restored structure is dominating, which is consistent with the Burgers vector of the AC+AB.

3.4. Dominating deformation mechanism

The shearing mechanism is represented by stacking-fault configuration and core structure of dislocation inside the precipitate’s microstructure. The final stacking-fault population
of crept alloy was investigated, which helped explain the observed deformation debris. 

However, in terms of the physics-based, yield-strength model, the intermediate stacking-fault configuration was more important than the final state, and it was related to the energy barrier of the deformation process.

According to our calculation, APB-like stacking fault or CSF stacking-fault ribbon is the major hardening mechanism. As a result, alloys with \( \gamma'' \) as the majority precipitate are guaranteed to have sufficient yield strength, although ISF is the dominant stacking-fault configuration in the final state of the crept alloy.

Dislocation structures associated with the stacking-fault ribbons inside realistic microstructure could be \( \frac{1}{2}\langle110\rangle \) full dislocation, \( 1/3\langle112\rangle \) super dislocation, or \( 1/6\langle112\rangle \) partial dislocation. These dislocation core structures and intermediate stacking-fault ribbon are used as input parameters of the fast-acting yield strength in Chapter 5.

3.5. Misfit strengthening

Misfit strengthening is one of the major strengthening effects of the microstructure with coherent precipitates. In 718-type superalloys, both \( \gamma'' \) and \( \gamma' \) particles provide misfit strain, but the misfit strain of the \( \gamma'' \) phase is relatively larger. In addition, since the \( \gamma'' \) phase is the dominant precipitate of 718-type superalloy, the misfit strengthening of the \( \gamma'' \) phase should be considered in a deformation model.

Due to the lower symmetry of the \( \gamma'' \) phase, the misfit strain field of a \( \gamma'' \) particle no longer shows three-fold rotational symmetry. As a result, the interaction between the misfit stress field and a full dislocation varies with the direction of Burgers vector. This is
totally different from the case in which a $\gamma'$ particle interacts with full dislocations. Since the misfit strain field has a three-fold rotational symmetry, a $\gamma'$ particle interacts with any full dislocation in an identical way, which results in a unique misfit strengthening to any equivalent slip system.

In this part, the complexity of the interaction between the $\gamma''$ misfit strain field and dislocations is revealed by the phase-field simulation of micro-elasticity. Two scenarios are investigated, which shows how the interaction varies with the direction of Burgers vector while its magnitude is fixed.

**Interaction between misfit stress field and AC+AB dislocation group**

In this scenario, an AC+AB dislocation group interacts with the three variants of the $\gamma''$ phase. Consequently, the interactions related to the Cδ and the Bδ are also calculated since the Cδ and the Bδ are created during the shearing process in a 718-type microstructure.

In every variant of the $\gamma''$ phase, a positive interaction energy density is observed, which implies a repulsive misfit force from the $\gamma''$ particles. The repulsive force force to the Cδ and the Bδ implies the shearing process of AB+AB slows down due to the existence of the misfit stress.
Figure 73. The interaction between the Variant 1 of the $\gamma''$ phase and the dislocations. The interaction energy density is plotted and represents a repulsive force.

Figure 74. The interaction between the Variant 2 of the $\gamma''$ phase and the dislocations. The interaction energy density is plotted and represents a repulsive force.
Figure 75. The interaction between the Variant 3 of the $\gamma''$ phase and dislocations. The interaction energy density is plotted and represents a repulsive force.

*Interaction between misfit stress field and CA+CB dislocation group*

In this scenario, an CA+CB dislocation group interacts with the three variants of the $\gamma''$ phase. Consequently, the interactions related to the $A\delta$ and $B\delta$ are also calculated since the $A\delta$ and $B\delta$ are created during the shearing process in a 718-type microstructure.

In every variant of the $\gamma''$ phase, a negative interaction energy density is observed, which implies an attractive misfit force from the $\gamma''$ particles.

Although the CA+CB dislocation group has the same magnitude of the Burgers vector as the AC+AB of the previous scenario, the sign of the interaction energy is reversed. This implies that the CA+CB is easier to cut into the $\gamma''$ particles since the misfit stress attracts...
the CA+CB into the $\gamma''$ particles. The attractive force force to the $A\delta$ and the $B\delta$ implies the shearing process of CA+CB accelerates due to the existence of the misfit stress.

Figure 76. The interaction between the Variant 1 of the $\gamma''$ phase and dislocations. The interaction energy density is plotted and represents an attractive force.
Figure 77. The interaction between the Variant 2 of the $\gamma''$ phase and the dislocations. The interaction energy density is plotted and represents an attractive force.

Figure 78. The interaction between the Variant 3 of the $\gamma''$ phase and the dislocations. The interaction energy density is plotted and represents an attractive force.
3. 6.  Composite particle formation: an aspect of the elastic energy

In the previous parts, only separate $\gamma'$ and $\gamma''$ particles were considered, and $\gamma'+\gamma''$ composite particles were ignored. However, recent experimental observations have shown strong co-precipitation processes of the $\gamma'$ and $\gamma''$ phases under certain heat treatment conditions [85].

Figure 79. The electron microscopy observation of the composite particles: (a) the cubic-like composite particle[76]; (b) the hamburger-like composite particle[86]. Generally, the cubic-like particle is of 0.1 um in size, while the length scale of the hamburger-like particle is finer, which is ~10nm.

Besides the separated $\gamma'$ and $\gamma''$ precipitates, large amounts of composite precipitates with two major morphologies have been observed, i.e., cubic-like and hamburger-like. For the cubic-like composite particles, as shown in Figure 79(a) [76], six surfaces of a cubic $\gamma'$ particle are covered by $\gamma''$ precipitates, while for the hamburger-like composite particles, as shown in Figure 79(b) [86], only two parallel surfaces of $\gamma'$ are covered by $\gamma''$. 
precipitates, and all of the particles have a disk-like shape. In some cases $\gamma' | \gamma''$ composite particles dominate, while, in other cases, the $\gamma'' | \gamma' | \gamma''$ configuration dominates. In general, the cubic-like composite particles have an average size of 0.1 $\mu$m, while the hamburger-like composite particles have an average size of $\sim$10 nm.

When the majority of precipitates are composite particles, the critical questions concerning the precipitation process are: (a) When are composite particles favored over separated $\gamma'$ and $\gamma''$ particles? and (b) Do the two types of composite particles share the same formation mechanism?

It is well known that the coherency elastic strain energy minimization may dominate the morphology of coherent precipitates\[87\]. For example, disk-like $\gamma''$ precipitates and cuboidal $\gamma'$ precipitates with \{001\} habit planes are all determined by the elastic anisotropy and the coherency elastic strain energy minimization. In particular, the aspect ratio of the $\gamma''$ precipitates keeps increasing during the coarsening\[82\], indicating the dominance of the elastic strain energy over the interfacial energy. Thus, it is nature to attribute the formation of the composite precipitate configurations to the elastic interactions. Indeed, as will be shown below, the elastic interaction energy favors the existence of the composite particle configuration. Whether the cubic-like or hamburger-like composite structure will form depends on the nucleation sequence. When the $\gamma'$ nuclei first, a cubic-like morphology is preferred. When the $\gamma''$ nuclei first, a hamburger-like morphology is more likely to occur. Further analysis shows that the elastic
interaction energy of a hamburger-like structure is sensitive to the orientation relationship between the γ′ and γ″ phases.

**Total elastic free energy for the hamburger-like composite particles**

The formation of a composite particle can be explained by the evolution of total energy in a microstructure. In this study, a hamburger-like particle is arbitrarily built up, and the total elastic energy is calculated and compared. Since the totally chemical free energy is supposed to be independent of the spatial distribution of the phases and the interfacial energy is neglected, the total energy change is assumed to be determined by the elastic energy term only.

Before calculating the total elastic energy term, the stress field of the hamburger-like composite particle, as a function of volume ratio is determined, which provides an insight of how the elastic interaction varies locally. The volume ratio is characterized as b/a, which is defined in Figure 80.
Figure 80. The stress field of the hamburger-like composite particle, as a function of the volume fraction of the $\gamma'$ phase and the space coordination. We adjust the $b/a$ ratio from 0 to 1, indicating from $\gamma''$ to $\gamma'$ particle, while the intermediate state is a hamburger-like composite particle. Here it is the case for the $\gamma''$ variant 1.

It should be mentioned that the $\gamma''$ phase itself prefer to form a disk-like particle since misfit strain is larger along the disk plane norm than along other direction. As a result, in order to reduce the elastic energy, the disk plane of $\gamma''$ prefers to contact with $\gamma'$ particle. Misfit strain of $\gamma''$ and $\gamma'$ along the norm direction compensate each other. When the contacting surface is improper, much higher energy will be induced.

In Figure 80, the misfit stress $\sigma_{11}$, $\sigma_{22}$, and $\sigma_{12}$ are shown. In the case of pure $\gamma''$ phase, very high positive stress level is obtained near the particle. In the case of pure $\gamma'$ phase,
stress field with a little negative value is obtained near the particle. Although the stress field $\gamma'$ phase is weak, when $b/a=0.5$, the stress field of $\gamma''$ phase is largely suppressed. In Figure 81, based on the stress field calculation, the total elastic energy is calculated as a function of $b/a$ ratio.

![Figure 81](image.png)

**Figure 81.** The total elastic energy is calculated as a function of the $b/a$ ratio. There are two lines in this figure. The red line corresponds to a direct mixture of the $\gamma'$ and $\gamma''$ phases under the given volume fractions, where the elastic interaction is neglected. On the black line, the elastic interaction between the $\gamma'$ and $\gamma''$ is considered.

There are two lines in this figure. The red line, corresponds to a direct mixture of $\gamma'$ and $\gamma''$ phases under given volume fractions, where the elastic interaction is neglected. On the blue line the elastic interaction between $\gamma'$ and $\gamma''$ is considered. Mixture rule is followed by the elastic field interference. There is an obvious gap between these two lines, which
means the composite particle is elastically preferred compared with separated particles. This helps to answer why the composite particle is of a large amount in TEM observations.

**Variant selection of the hamburger-like composite particle**

In the previous section, a proper contacting surface is chosen to construct the hamburger-like composite particles. When other the contacting surface normal is selected, much higher energy will be induced.

![Figure 82](image)

Figure 82. The stress field of the “improper” hamburger-like composite particle, as a function of the volume fraction of the $\gamma'$ phase and the space coordination. We adjust the b/a ratio from 0 to 1, indicating from $\gamma''$ to $\gamma'$ particle, while the intermediate state is a hamburger-like composite particle. Here it is the case for the $\gamma''$ variant 1.
In Figure 82, the misfit stress $\sigma_{11}$, $\sigma_{22}$, and $\sigma_{12}$ are shown. In the case of pure $\gamma''$ phase, very high positive stress level is obtained near the particle. In the case of pure $\gamma'$ phase, stress field with a little negative value is obtained near the particle. In this case, the magnitude of stress field is not efficiently decreased inside the $\gamma'$ phase, especially for $\sigma_{22}$.

In Figure 83, there are two lines in this figure. The red line corresponds to a direct mixture of $\gamma'$ and $\gamma''$ phases under given volume fractions, where the elastic interaction is neglected. On the blue line, the elastic interaction between $\gamma'$ and $\gamma''$ is considered. There is an obvious gap between these two lines, which indicates that the “improper” composite particle is elastically NOT preferred compared with separated particles. In this morphology, if the $\gamma''$ variant 1 is replaced by variant 2, the new composite particle will be elastically preferred, similar to the result in Section 5. Again, the contacting surface selection is a result of 3-fold rotational symmetry lost. The experiment observation confirmed such variation selection.
3.7. Discussion

The deformation mechanisms revealed by the phase field simulations is consistent with the concurrent experimental observations [88]. For example, APBs are not observed in the γ” particles and no stacking faults are observed in the matrix either. At lower temperature, isolated stacking faults have been observed, which is highly possible to be SISF. At the intermediate temperatures, the SESF is found to be the dominating deformation mechanism. At high as well as intermediate temperatures, extensive microtwin have been observed. Meanwhile, an abundance of <112> type dislocations has been observed in IN718, whereas there are few stacking faults in the matrix. Together
with these characteristics, perfect stacking sequence in the $\gamma$ matrix requires the Burgers vector of the dislocations to be $n/2<112>$ type.

In the deformation modes of $\gamma''$ phase proposed in previous literature, only pair and quadruplet of dislocations with identical $1/2<110>$-type Burgers vector were considered, with a pair restoring the perfect stacking sequence in one $\gamma''$ variant and a quadruplet restoring the perfect stacking sequence in the other two variants [2]. These are obviously not the operating deformation modes in IN718. Since ISF energy is ultra low ($\sim 2.3\text{mJ/m}^2$) and the SF-ribbons are also low-energetic configurations, the CA+BA (i.e., the $1/2<112>$ type) dislocation group could be the weak deformation mode of the $\gamma''$ phase in IN718.

Since the ISF energy is ultra low according to the DFT calculation, twinning could be another weak deformation mode inside the $\gamma''$ particles, as well as inside the $\gamma$ matrix. Indeed, microtwin can be created with ISFs in successive $\{111\}$ atomic layers without the requirement of re-ordering, which is different from twinning in $\gamma'$. In order to decide the deformation pathway of twinning in $\gamma''$, the energy barrier for the twin propagation needs to be determined.

For the composite particles, it should be mentioned that, there could be other effects, such as very low interfacial energy between $\gamma'$ and $\gamma''$, contribute to the stabilization of the composite precipitates. A microstructure evolution investigation is necessary to explain how different mechanisms contribute to the formation of composite microstructure[39].
Furthermore, a deformation modeling is required to check whether the composite particle decrease or enhance the yield strength and what is the mechanism for the influence [39].

3.8. Summary

(1) The dislocation and stacking-fault configurations associated with several different dislocation configurations were identified by the DFT-based, phase-field simulations. According to the simulation, it is easy for the AC+AB dislocation group to be active. This dislocation configuration is different from that predicted by the APB-type model in the literature [2]. This is a critical piece of information that is needed for the development of a fast-acting, yield-strength model of the alloy. Since these configurations are transient and do not exist in the final deformation microstructures, it is extremely difficult to determine what they are by an experimental study alone.

(2) Assuming that the observed dislocation configurations in the deformed alloy are those that have extremely low activity, the pinning effect to <112>-type dislocations explains the recent TEM observation on IN718 superalloy in which the <112>-type dislocation was found to be dominant. This pinning effect is significant irrespective of the type of input dislocation group that is active, and it has been observed in both individual particle deformation and realistic microstructure deformation.

(3) The partial dislocation loops created by the stacking-fault transformation can expand through the matrix when the applied stress favors the interaction with other γ" precipitates and reacts with other dislocations. However, in a realistic microstructure, the emitted dislocation loops will be pinned by the γ’ particles due to the high CSF energy in
the $\gamma^\prime$ phase. The $\gamma^\prime$ particles also pin the emitted particle dislocation loops, because the $1/6\langle11\bar{2}\rangle$ displacement corresponds to high-energy, unstable SFs. When the $\delta C$ loop expands, it is pinned by Variant 1 and Variant 3 of the $\gamma^\prime$ phase, while shearing of these precipitates would create high-energy, unstable CSF. When the $\delta B$ loop expands, it will be pinned by Variant 2 and Variant 3 of the $\gamma^\prime$ phase for the same reason. For the already faulted $\gamma^\prime$ particles, the situation becomes much more complicated.

(4) In addition to the final dislocation and stacking-fault configurations, the deformation mechanisms that determine the strength and creep rate are related to the intermediate, highly-energetic stacking-fault ribbon. These intermediate stacking-fault ribbons guarantee that the $\gamma^\prime$ phase is still a strong phase in terms of deformation hardening.

(5) According to the phase field simulation, partial dislocation nucleation may or may not be energetically preferred, depending on the direction of the input dislocation. Since the partial dislocation nucleation controls the formation of the stacking ribbon, deformation anisotropy is predicted, which means that equivalent slip systems of the matrix experience different hardening effects from different variants of the $\gamma^\prime$ phase.

(6) The formation of composite particles and their morphologies depend on the elastic interaction between the different $\gamma^\prime$ and $\gamma^\prime$ phases. Due to the tetragonal symmetry of the $\gamma^\prime$ phase, there are proper and improper configurations of $\gamma^\prime/\gamma^\prime$ composite particles. In the proper configuration, total elastic energy is less than that of the isolated phases of $\gamma^\prime$ and $\gamma^\prime$. 

131
Chapter 4: Deformation Mechanisms of the $\gamma/\gamma'$ Microstructure in Superalloys

In this part, we investigate the hardening mechanism in superalloys with $\gamma/\gamma'$ microstructure. In Figure 84, the TEM picture of Co-based superalloy shows cubic-like $\gamma'$ particles. The formation of cubic-like particle morphology in the Co-based superalloy requires an extended aging period and a specific composition.

Figure 84. A TEM picture of the cubic-like $\gamma'$ particles of a Co-based superalloy.

The $\gamma'$ particles can be either looped or sheared, depending on physical parameters such as line-tension, stacking-fault energy and lattice friction, and the microstructure features such as particle size, inter-particle distance and local curvature of the particle.
morphology. These features are controlled by chemical composition, heat treatment, work hardening, applied load and temperature.

Figure 85. A TEM picture of the APB and SISF configurations in the Co-based superalloys [21].

In Figure 85, an APB shearing is shown in the CoNi-base superalloy. APB is created by any full dislocation which cuts through a perfect crystal. In most cases, the APB energy is too high that a large area of APB debris is forbidden. The APB shearing is usually accompanied with a pair of full dislocations which have the identical Burger vector and restore the perfect crystal. During this cutting process, an APB ribbon is created between these two full dislocations.

Besides the formation of the APB ribbon, there are other possible ribbon configurations which appear during a cutting process. In order to understand the stacking ribbon configurations, the GSF potential energy has been calculated in Chapter 2. Indeed, any stable configuration (stacking fault) on the GSF surface can be produced in a crystal in the form of ribbon during a cutting process. For example, besides APB, the SISF ribbon has also been widely observed. The high energetic stacking fault ribbon, such as the CSF
ribbon, is hard to be observed in the experiment since the ribbon width is controlled by the stacking-fault energy. The equation that estimates the ribbon width is:

\[
\frac{\alpha g \overrightarrow{b_1} \cdot \overrightarrow{b_2}}{d} = \Delta \Gamma
\]

This equation describes the force balance between two dislocations with Burgers vectors \( b_1 \) and \( b_2 \). The left-hand expression corresponds to the elastic interaction between two dislocations. This interaction could be repulsive or attractive depending on the angle between \( \overrightarrow{b_1} \) and \( \overrightarrow{b_2} \). The \( \alpha \) is a scaling factor which varies with the line direction, the angle between two Burgers vectors, and Poisson’s ratio. The \( G \) is the shear modulus. The \( \Delta \Gamma \) is the stacking-fault energy difference inside and outside ribbon (\( \Delta \Gamma_{\text{in}} - \Delta \Gamma_{\text{out}} \)). The \( d \) is the ribbon width. According to the above equation, with the increment of positive stacking-fault energy difference, the ribbon width decreases. Meanwhile, dislocation distance increases with shear modulus when \( \overrightarrow{b_1} \cdot \overrightarrow{b_2} \) has a positive sign, which is a result of larger repulsive force.

Besides the stacking fault ribbon which moves through the particle and disappears in the final state of the deformation, a large area of debris stacking fault can also be formed in the final state in many scenarios. For example, when the stacking-fault energy is not so high, or the applied stress is high enough, or the local curvature of a particle is large, a large area of stacking fault can be observed. When the stacking-fault energy is too high, it is impossible for cutting process to happen. Instead, the Orowan looping happens and the inter-particle distance controls the deformation mechanism.
The stacking-fault energy is the key parameter of a physics-based deformation mechanism model. It has been systemically investigated in several alloys through experiments and the DFT method. In Chapter 2, according to a recent work by Michael Titus at UCSB, the stacking-fault energy as a function of composition has been plotted [21]. The variation of the APB energy follows a mixture law. At the composition ends of Ni-based and Co-based superalloys, the APB energy is relatively high. At the composition of the CoNi-based superalloy, however, the APB energy is significantly lower. The variation of the SISF energy is more monotonic, and the SISF energy is low in the Ni-based superalloy [21].

Since APB and SISF do not follow the same rule of composition dependence, the variation of the precipitate hardening mechanism could be a complex function of the composition. In order to predict the deformation mechanism, a phase-field deformation simulation is performed to investigate the interaction between the dislocations and the γʹ particle. The composition dependences of the deformation mechanism and the stacking fault configuration are revealed which is compared with TEM observations directly.

Then, a stabilized combination of different stacking fault configurations in the triangular and the hexagonal cross-sections of the γʹ particle are predicted. It is shown that the particle morphology and the elastic energy are the important factors that decide the shearing process besides the composition.

Some parameters other than the stacking fault energies are listed in Table 5.
<table>
<thead>
<tr>
<th>Name of parameter (unit)</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burgers vector (nm)</td>
<td>$a$</td>
<td>0.146</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>$\nu$</td>
<td>0.3</td>
</tr>
<tr>
<td>Shear modulus (GPa)</td>
<td>$\mu$</td>
<td>150</td>
</tr>
</tbody>
</table>

Table 5. Some physical parameters used in this chapter.

4.1. Deformation of spherical particles

*Deformation by $\frac{1}{2}<110>$ (AB) single dislocation*

First of all, an AB dislocation is set to interact with a spherical $\gamma'$ particle. The AB dislocation movement on the (111) plane and the resolved shear stress is 600 MPa. The phase field simulation results related with the AB single are displayed for Ni-base superalloy (Figure 86), CoNi-based superalloy (Figure 87 and Figure 88), and Co-based superalloy (Figure 89). Three frames of deformation process are displayed for each composition, and describe (1) onset of interaction between dislocation and particle boundary, (2) configuration of dominating hardening mechanism, (3) dislocation debris and stacking fault debris.
Figure 86. A deformation process is simulated by the phase-field approach when an AB single dislocation interacts with a $\gamma'$ particle in a Ni-based superalloy. The Orowan looping happens which is due to the high APB energy.

Figure 87. The early stages of a deformation process are simulated by the phase-field approach when an AB single dislocation interacts with a $\gamma'$ particle in a CoNi-based
superalloy. The APB shearing happens which is a result of the relatively low APB energy.

Figure 88. The later stages of a deformation process are simulated by the phase-field approach when an AB single dislocation interacts with a γ' particle in a CoNi-based superalloy. The debris structure is APB due to the relatively low APB energy.

Figure 89. A deformation process is simulated by the phase-field approach when an AB single dislocation interacts with a γ' particle in a Co-based superalloy. The Orowan looping happens which is due to the high APB energy.
In the first frames for each composition, curvature of dislocation is increased at the particle boundary. At the same time, line-tension force tends to straighten the dislocation line in order to minimize the dislocation line energy. The line-tension force and applied stress would drive particle shearing if stacking-fault energy is relatively low. Otherwise, Orowan looping happens and dislocation percolates through the matrix.

In the simulations, line energy is controlled by core energy (expressed by GSF surface), elastic energy and gradient energy. Since at each composition the elastic energy and gradient energy are set to be identical, stacking-fault energy and core energy (also expressed by GSF surface) are the only parameters which decide the selection between looping and shearing. As a result, in the phase field simulation, this composition dependence of deformation mechanism is represented through GSF surface.

In Ni- and Co- based alloys, Orowan looping is observed because firstly APB energy is relatively high, and secondly the inter-particle distance is 342 nm and ~2 times of the particle size.

In contrast, in CoNi- based superalloy, AB dislocation cuts through particle and APB debris is left. APB energy in CoNi- based superalloy is only 100 mJ/m², which is far smaller than that of the Ni-based alloy (~240 mJ/ m²) or the Co-based alloy (~160 mJ/ m²). Although AB single is easy to be active, there is still a question: is APB single dislocation the minimal unit that was observed in the experiments. In principle, another AB dislocation could follow up and restore the perfect crystal structure of $\gamma'$. AB pair is
more likely to happen since APB ribbon should always be a weaker mechanism than the creation of APB debris. Consequently, in experiments AB dislocations should always be observed in pairs. However, when the APB energy is low and the two AB dislocations are weakly coupled, CRSS of AB pair will be very close to that of single AB. Then AB is the semi-minimal unit that represents deformation mechanism of <110>-type cutting process.

*Experimental observations of deformation by $\frac{1}{2}<110>$ (AB) single dislocation*

ABP debris created by full dislocation has been observed in crept CoNi-based alloy. According to Mikael’s work [21], the dislocation which is related to APB debris is exactly $\frac{1}{2}<110>$ type. A demonstration of the observation is shown in Figure 90, where green area displays APB debris. This figure gives a conceptual explanation of what happened in the TEM picture. The green area will later dominate the entire cross section if in-plane cutting continues. However, the cross slip has been widely observed in TEM pictures, which could be due to Kear-Wilsdorf lock. As a result, APB debris will only occupy some area of particle cross section while the remaining particle area stays perfect. In our simulation, only APB shearing on one of (111) planes is considered. Neither cross slip nor APB on (100) plane (KW lock) is investigated in this work.
Figure 90. A 3-D plot [21] shows how an AB dislocation interacts with a cubic-like $\gamma'$ particle on (111) plane. The (111) cross section is triangular. The APB area is displayed in yellow color. The blue color indicates the area which has not been sheared.

It should be mentioned that in Figure 90, the shearing plane is a triangular cross section of a cubic particle. The effect of the local high curvature at the edge of the cubic is not considered in this conceptual demonstration. However, as will be shown in later simulations where the effect of the particle boundary curvature is considered, co-existence between stacking faults will happen at proper loading condition.

**Deformation by $\frac{1}{2}<112>$ (AB+AC) dislocation group**

Besides single dislocation and pair of full dislocations, $<112>$-type dislocation group is another popular configuration inside superalloys with $\gamma/\gamma'$ microstructure. According to observations in Ni-based superalloys [10], $<112>$-type dislocation group creates SESF, which is accompanied with chemical re-ordering. The extrinsic stacking fault is formed so that intermediate high energetic CSF state is avoided. The energy of extrinsic stacking fault has been investigated by molecular dynamics which shows a significant energy
reduction when the intrinsic stacking fault transform into extrinsic one. During the formation of SESF, SISF was thought to be created as a ribbon of the intermediate state. Since the activation of re-ordering process strongly depends on composition and service temperature, deformation mechanism without the assistance of re-ordering will be a more general case. This is important for alloys which serve at relatively low temperature or which have elements of low diffusivity.

Figure 91. The GSF surfaces of the $\gamma'$ phases shows the deformation pathway of the AB+AC dislocation shearing.

The formation mechanism of SISF debris needs to be investigated which is the focus of this part of work. When chemical re-ordering is weak, SESF is hard to be created.
Instead, SISF will be created in a large amount. According to deformation process in Figure 93, the formation of SISF is followed by the creation of APB. Before SISF formation, APB ribbon is formed which is the critical stage.

Figure 92. The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a γ' particle in a CoNi-based superalloy. The APB shearing happens which is a result of the relatively low APB energy.
Figure 93. The Frame 4 of the above simulation is enlarged in order to display the detailed dislocation and the stacking fault configurations.

Figure 94. The later stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a $\gamma'$ particle in a CoNi-based superalloy. The APB is created as the debris due the relatively low APB energy.
The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a $\gamma'$ particle in a Co-based superalloy. The SISF shearing happens while an APB area is absent, which is a result of the relatively high APB energy.

The Frame 3 of the above simulation is enlarged in order to display the detailed dislocation and the stacking fault configurations.

Figure 95.

Figure 96.

The Frame 3 of the above simulation is enlarged in order to display the detailed dislocation and the stacking fault configurations.
Figure 97. The later stages of a deformation process are simulated by the phase-field approach when an AB+AC group interacts with a γ' particle in a Co-based superalloy. The APB is created as the debris while the Aδ dislocation loop is left at γ/γ' boundary, due the relatively high APB energy.

Although an intuitive explanation could be that lower SISF energy is related to a larger area of SISF debris, our simulation does not support this guess. In this work, we investigated three alloys with different composition: Ni-based, CoNi-based and Co-based. Our simulation shows that SISF debris is created in the alloy with highest SISF energy. This unexpected result is finally explained by dominating deformation mechanism. According to our simulation, SISF energy is not the key factor that controls the width of SISF debris. Instead, APB cutting is confirmed to be dominating strengthening configuration which decides whether a narrow ribbon or large area of SISF would be created.

In this part, we performed DFT-based phase field simulation in order to predict stacking fault configuration and dislocation configuration related with this shearing process. According to the configuration of GSF surface, SISF is assumed to be created by
½<112> dislocation group when it cuts through a perfect γ’ particle. As a result, AB+AC dislocation group is set to interact with a spherical γ’ particle inside γ phase matrix. Since the focus of this work is to understand the effects of chemical composition and applied stress, the particle cross section is set to be disc-like so that the local curvature effect of particle boundary can be avoided. The particle boundary curvature will be investigated in details later.

In this simulation, AB+AC dislocation moves on (111) plane and resolved shear stress is 600 MPa. The simulation results are display for CoNi-based superalloy (Figure 92, Figure 93 and Figure 94) and Co-based superalloy (Figure 95, Figure 96 and Figure 97). For each composition, three stages of deformation process are displayed in order to describe typical deformation stages. The typical deformation stages are (1) increment of dislocation curvature which indicates the onset of interaction between dislocation and particle boundary, (2) configuration of dominating hardening mechanism which could be roughly classified into Orowan looping or stacking fault shearing, (3) dislocation debris and stacking fault debris.

In the first frame for each composition, dislocation curvature increases when it interacts with the particle boundary. Basically, if the line energy of curved AB+AC group is higher than the stacking-fault energy created by the straightened dislocation line, stacking fault shearing is dominating. Otherwise, Orowan looping happens. In the simulation, line energy is controlled by core energy, elastic energy, and gradient energy, when the elastic energy and gradient energy are set to be identical for each composition. As a result,
stacking-fault energy and core energy vary with composition and are parameters which decide the selection between looping and shearing at each composition. Indeed, stacking-fault energy and core energy are both represented by GSF surface which is a function of composition in the simulations.

As will be shown the analytic model, although SISF has lower energy in Ni-based superalloy than that in Co-based superalloy, SISF debris is still created in Co-base superalloy, while in Ni-based superalloy only Orowan looping happens. This result will imply that final debris in the crept alloy is not a satisfactory condition for determining the dominating deformation mechanism.

According to phase field simulations in Figure 93 and Figure 96, shearing processes varies with composition. According to the phase field simulation, the dominating stacking fault configuration is primarily APB ribbon and secondarily APB shearing, no matter whether SISF debris or APB debris is created.

Due to ultra-high APB energy, Orowan looping happens in the Ni-based alloy. In the CoNi-based alloy, SISF ribbon is formed, and a large area APB is also created due to its low energy. An upcoming AB+AC groups will finally restore the perfect crystal structure, and a multi ribbon structure will be formed.

In Co-based superalloy, since ABP energy is higher, it cannot be formed as deformation debris. Only SISF and a partial dislocation are left as debris. Upcoming dislocations will not remove this SISF or from APB until perfect crystal structure or another SISF is created.
Experimental observations of deformation by $\frac{1}{2}<112> (AB+AC)$ dislocation group in the CoNi-based superalloy

Our simulation in CoNi-base superalloy provides an alternative explanation to APB debris. Although in Mike’s work the dislocation which is associated with APB debris is a $\frac{1}{2}<110>$ type, our simulation shows that $\frac{1}{2}<112>$ type dislocation group can also create APB inside $\gamma'$ particles. The proposed explanation is shown in Figure 98, where APB debris is displayed with green color. This figure gives a conceptual prediction of what would happen in the CoNi-based superalloy when $\frac{1}{2}<112>$ group is active. The APB debris will later dominate the entire cross section if in-plane cutting continues. Although cross slip has been widely observed in TEM pictures which could be due to Kear-Wilsdorf lock, there is no investigation of cross slip of $<112>$ type dislocation inside CoNi-based superalloy. If cross slip happens, APB debris will only occupy some portion of particle cross section while the remaining cross section area stays not cut. In our simulation, only APB shearing on one of $(111)$ planes is considered.
Figure 98. A 3-D plot [21] shows how an AB+AC group interacts with a cubic-like γ’ particle on the (111) cross section. The APB area is displayed in the yellow color. The blue color indicates the area which has not been sheared.

It should be mentioned that the particle cross section in Figure 98 is no longer disk-like, but a triangular cross section which belongs to one of cross section types of a cubic particle. The effect of the local high curvature at the cube edge has not been considered here. However, in later simulations, effect of particle boundary curvature will be investigated, and co-existence between stacking faults as well as stabilized stacking fault island will be revealed at the proper condition.

**Experimental observations of deformation by \( \frac{1}{2} \langle 112 \rangle \) (AB+AC) dislocation group in the Co-based superalloy**

Our simulation in Co-base superalloy provides an explanation to SISF observed by TEM. In Mike’s work the dislocation which is related to SISF ribbon is a \( \frac{1}{2} \langle 112 \rangle \) type. A demonstration of the dislocation and stacking fault configurations is shown in Figure 99, where SISF is displayed with blue color. This figure gives a conceptual prediction of
what would happen in the Co-based superalloy when ½<112> group is active. During the
defformation process, 1/3<112> super-dislocation cutting through the particle and leaves
SISF debris. At the same time, a 1/6<112> type partial is left and loops around the
particle in order to avoid high energetic APB area. The SISF debris will later dominate
the entire cross section if in-plane cutting continues. At higher temperature, or when the
alloy contains elements with high diffusivity, an upcoming ½<112> dislocation group
will create SESF with the assistant of chemical re-ordering. In that case, shearing will
happen on two adjacent planes. In our simulation, only APB shearing on one of (111)
planes is considered.

Figure 99. A 3-D plot [21] shows how an AB+AC group interacts with a cubic-like γ'
particle on the (111) cross section. The SISF area is displayed in the green color. The
blue color indicates the area which has not been sheared.

Again, the particle cross section in Figure 99 is no longer disk-like, but a triangular cross
section which belongs to one of cross section types of a cubic particle. The effect of the
local high curvature at the cube edge has not been considered above. In the following
simulations, particle boundary curvature will interact with dislocation line in two types of cross section. At proper loading condition, and co-existence between stacking faults as well as stabilized stacking fault island will be revealed.

4.2. Formation of SISF island

(111) cross section of cubic-like γ' particle

Figure 100. A 3-D plot shows two types of the (111) cross sections of a cubic-like γ' particle.

In order to investigate the effects of particle boundary curvature on the deformation mechanism, realistic cross section of γ' particle needs to be considered in the deformation simulations. In Figure 100, two types of the (111) cross section are shown for a cubic particle. The first one is triangular and the second one is hexagonal. Triangular cross section possesses relatively higher local curvature at corners. At the same time, the hexagonal cross section has lower local curvature at corners. Figure 100 only gives a rough description of morphology symmetry for each cross section. In Figure 101 and Figure 102, the sharp corners are relaxed by using phase-field microstructure evolution
package. Besides the initial morphology, the evolution considered misfit stress which is a key factor that influences the corner curvature. The misfit stress of $\gamma'$ particle follows the data from [89]:

$$\epsilon^* = \begin{bmatrix} -0.003 & 0 & 0 \\ 0 & -0.003 & 0 \\ 0 & 0 & -0.003 \end{bmatrix}$$  \hspace{1cm} (26)$$

Figure 101. A triangular (111) cross section of the $\gamma'$ phase evolves, which is simulated by the phase-field approach.
It is obvious that triangular cross section has much higher local curvature. As a result, deformation of triangular cross section tends to be more inhomogeneous. At locations with higher curvature, the driven force by line tension is high and particle shearing is easy to happen. Meanwhile, at low curvature position, stacking fault and lattice friction dominates. The stacking-fault energy prohibits shearing if it was increased by cutting process. When the stacking-fault energy is decreased, the cutting process is preferred. An equilibrium state can be reached when all the forces related with dislocation line balance each other. For a circular dislocation loop, the formation energy of a stacking fault island can be balanced by external work, which can be expressed as:

\[
E_{S.F.,in} - E_{S.F.,0} + E_{LT} = W_{ext}
\]  
\[
E_{S.F.,in} = \Gamma_{ln}\pi r^2, E_{S.F.,0} = \Gamma_{ln,0}\pi r^2, E_{LT} = 2\pi r T
\]
\[ T = \frac{\mu b^2}{2} \frac{2-v}{2(1-v)} W_{\text{ext}} = \frac{\tilde{t}_{\text{ext}} \cdot \vec{b}}{d} d\pi r^2 \]  

(29)

Where \( E_{\text{S.F.,in}} \) is the total chemical energy inside the stacking fault island, and \( E_{\text{S.F.,0}} \) is the total chemical energy before the creation of island. \( \Gamma_{\text{in}} \) is the stacking-fault energy inside the island, \( \Gamma_{\text{in,0}} \) is the stacking-fault energy before the creation of island, and \( r \) is the radius of stacking fault island. \( E_{LT} \) represents line energy and \( T \) is the line tension. 

\( W_{\text{ext}} \) is the external work, which is done on a volume of \( d\pi r^2 \). \( d \) is the thickness of the material.

A future simplification of the expression gives a relationship among applied stress, stacking energy and local curvature:

\[ \tilde{t}_{\text{ext}} \cdot \vec{e}_b = \frac{\Delta \Gamma}{b} + \frac{\mu b}{r} \frac{2-v}{2(1-v)} \]  

(30)

Where \( \vec{e}_b \) is the unit vector of Burgers vector and \( \Delta \Gamma = \Gamma_{\text{in}} - \Gamma_{\text{in,0}} \).

**Phase-field simulation of the SISF island formation**

According to the TEM observation by Michael Titus [21], besides the stacking fault ribbon, SISF island is also observed inside APB debris of \( \gamma' \) particles.

SISF island may play as a precursor to an important deformation mechanism in superalloy – microtwin. Microtwin has been widely observed in previous TEM works [18]. It possesses significantly higher creep rate compared with in-plane shearing, since the microtwin shear deformation happens in several atomic planes simultaneously.
Figure 103. The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a $\gamma'$ particle in a Co-based superalloy. The cross section is triangular. The AB dislocation has already cut through the particle. The APB and SISF are observed to coexist during the deformation.

Figure 104. The final stage of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a $\gamma'$ particle in a Co-based superalloy. The cross section is triangular. The APB and SISF coexist in a stable configuration.
Figure 105. The early stages of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a $\gamma'$ particle in a Co-based superalloy. The cross section is hexagonal. The AB dislocation has already cut through the particle. The APB and SISF are observed to coexist during the deformation.

Figure 106. The final stage of a deformation process are simulated by the phase-field approach when an AB+AC group interact with a $\gamma'$ particle in a Co-based superalloy. The cross section is hexagonal. Only the SISF exists in the stable configuration.
According to the previous deduction of the expression which connects stacking-fault energy, curvature and applied shear stress, if we remove the applied stress term which is absent in the observed sample, the expression displays a balance between dislocation line tension and stacking-fault energy difference:

$$\tau_{ext} \cdot \hat{e}_b = \frac{\Delta \Gamma_{SISF-APB}}{b} + \frac{\mu b}{r_{local}} \frac{2-\nu}{2(1-\nu)}$$  \hspace{1cm} (31)

In the absence of applied stress:

$$\frac{\Delta \Gamma_{SISF-APB}}{b} = -\frac{\mu b}{r_{local}} \frac{2-\nu}{2(1-\nu)}$$  \hspace{1cm} (32)

Since SISF island is formed by a partial dislocation which cuts through existing APB, the island shrinks firstly and then reaches an equilibrium configuration. According to this expression, it is clear that the existence of SISF island implies that SISF energy should be lower than APB energy (or the curvature is negative, which is impossible in the case), which was a basic assumption when SISF energy is calculated according to TEM observations. If SISF energy is higher than APB energy and the curvature is positive, then the total force on Aδ dislocation can never be balanced and the island shrinks until it disappears.

As is shown in the phase-field simulation in Figure 103 and Figure 104, the stable island is easily formed in triangular cross section. At the corners of triangular, due to the high local curvature of particle boundary, Aδ dislocation line shrinks and APB is created, while on the edge of the cross section, SISF is more stable. As a result, coexistence
between SISF and ABP happens in the γ’ particle happens, which corresponds to the island observed by TEM. It should be mentioned that once the dislocation loop expands into the matrix, the force field will be changed since both dislocation core energy and stacking-fault energy difference are significantly reduced.

![Diagram](image_url)

Figure 107. The stabilized shapes of the Aδ dislocation loop in the presence and absence of Poisson’s ratio.

In the hexagonal cross section, deformation is more homogenous, since the corner curvature is low. As a result, there is little chance for SISF and APB to coexist. The simulation results are shown in Figure 105 and Figure 106.

During the shearing process, SISF island is always non-spherical. Even if the initial loop is a perfect circle, as is shown in Figure 107, the final configuration is an ellipse. Indeed, the driving force on screw and edge dislocation segments are different, due to the existence of Poisson’s ratio.

As a result, the final dislocation configuration prefers higher line fraction of screw dislocation, which implies an ellipse shape. In Figure 107, a parametric study is
performed which shows how the final configuration varies with Poisson’s ratio. When Poisson’s ratio is trivial, the final configuration is an almost perfect circle.

The effect of Poisson ratio is also revealed at the beginning of shearing mechanism. In the triangular cross section, two of the three corners are sheared firstly. The reason is that screw dislocation has lower line energy, and the driven force of reshaping dislocation line prefers higher line fraction of screw dislocation. At these two corners, the edge dislocation segments, which is indicated by green arrows, is removed when the dislocation cuts through. After shearing at these corners, a very high line fraction of screw dislocation is formed.

In the hexagonal cross section, again, two of the six corners are sheared firstly. The reason for this phenomena is the same as in triangular cross section. The line energy depends on whether the dislocation is screw or edge and the final configuration prefers high line fraction of screw dislocation as is shown. It is interesting that simulated island configuration is consistent with TEM picture observed by Michael Titus, which means the Poisson’s ratio in the observed alloy is significant.

4.3. Stability of the SISF island

The previous simulation in Co-based superalloy shows a stable SISF island inside APB. The stability is strongly influenced by cross section geometry, that is, triangular or hexagonal.

Meanwhile, the chemical composition should be another significant factor which influences the stability of SISF island. In Chapter 2, GSF surfaces for γ’ phase in Ni-
based, CoNi-based and Co-based superalloys have been systematically investigated. Then these GSF surfaces are used as inputs to phase field simulation of deformation process. When other factors such as particle morphology, lattice friction, and elastic modulus are fixed, the phase field simulation can reveal how the stability of SISF island depends on alloy composition.

The phase field simulation in the Co-based superalloy has been performed, which reveals a stable SISF island inside APB under zero applied shear stress. Using the stable configuration in the Co-based alloy, SISF island evolution in other two alloys are also simulated. In both cases, there is no stable coexistence between SISF and APB.

Phase field simulation in Ni-based superalloy is shown in Figure 108. In this case, SISF island expands until APB area is completely consumed. As a result, the force from line energy and lattice friction is insufficient to balance the force of stacking-fault energy difference. After APB area totally disappears, the $A\delta$ dislocation line stops at the particle boundary, which is due to the effect of ISF energy in the matrix.

In CoNi-based alloy, the SISF area shrinks and finally disappears, since the stacking-fault energy difference between SISF and APB is small and is unable to balance the force from dislocation line curvature. The phase field simulation of this case is shown in Figure 109.
Figure 108. In the Ni-based superalloy, a deformation process is simulated by the phase-field approach when an initial dislocation configuration of the SISF+APB is applied. This initial configuration is stable in the Co-based superalloy. The APB area finally disappears due to the relatively high APB energy.

Figure 109. In the CoNi-based superalloy, a deformation process is simulated by the phase-field approach when an initial dislocation configuration of the SISF+APB is applied. This initial configuration is stable in the Co-based superalloy. The APB area gradually expands and will finally consume all the SISF area, which is a result of the relatively low APB energy.
4.4. Summary

Three aspects of particle shearing in the $\gamma/\gamma'$ microstructure were identified by the DFT-based phase field simulation.

(1) AB+AC shearing occurred in the Co-based and CoNi-based superalloys, and the stacking-fault/dislocation configuration in the crept alloys explain the TEM observations. In the Ni-based superalloy, AB+AC only induces Orowan looping since APB’s energy is very high. In the CoNi-based superalloy, the deformation debris was APB, while it was SISF in the Co-based superalloy. Although the deformation process in the three alloys was different, all of them were controlled by the high energetic stacking fault, APB. In addition to the final configuration, the phase field simulations also showed the stacking-fault ribbon during the deformation. For example, APB ribbon, CSF ribbon, and SISF ribbon are displayed in the contours of the crystalline energy. These contours revealed the core structure of the dislocation group so that an analytic model of CRSS for AB+AC shearing could be developed. Then, the analytic model can be used to answer the question concerning which stacking fault is dominant.

(2) The simulation showed that a large area of stacking-fault debris can be created without the assistance of chemical re-ordering. The phase-field simulation showed a large amount of SISF debris in the Co-based superalloy, although the SISF energy was relatively high. It was found that the balance between the stacking-fault energy and the elastic energy was the dominant mechanism that controlled the formation of SISF.
(3) The simulation showed the condition when the SISF island inside APB was stable. The stability of the SISF island depends on chemical composition, particle size, corner curvature, and dislocation line energy. According to the simulation, the SISF island easily was formed in the Co-based superalloy, while it was unstable in the Ni-based and CoNi-based superalloys even though the particle sizes were the same. Also, a parametric study showed that the shape of the SISF island depended on Poisson’s ratio.
Chapter 5: Fast-Acting Models of Superalloy Deformation

5.1. Fast-acting Orowan looping model

In superalloys with $\gamma/\gamma'$ microstructure, Orowan looping is one of the major mechanisms deciding the creep rate in the $\gamma$ matrix channel. The modes of looping mechanism include full dislocation ($\frac{1}{2}<110>$) looping, partial dislocation looping ($\frac{1}{6}<112>$) (de-correlation) and inactivity. Full dislocation is the most common configuration, especially when the inter-particle distance is comparable with or larger than particle size.

Besides full dislocation activation which is a common deformation mechanism, de-correlation activation is believed to be related to the easy formation of microtwin [10] inside superalloy. When de-correlation happens, a large area of ISF is created inside the matrix. When ISF is formed at several adjacent atomic layers, microtwin appears in the $\gamma$ matrix. What is more, the leading partial can cut into $\gamma'$ particles when the applied stress is high enough. This cutting process creates CSF inside the $\gamma'$ particle and an accompanied chemical re-ordering will transform CSFs from two adjacent atomic layers into an SESF, which is a microtwin precursor in the $\gamma'$ particle. As a result, de-correlation plays as a precursor to continuous microtwin throughout the entire crystal.

Besides particle size, channel width and Burgers vector, dislocation source distribution is another factor controlling where the activation happens and the final population of
dislocation configurations. Dislocation sources can be either rare throughout the crystal or densely distributed. In the latter case, looping mechanism is controlled by the average channel width. According to previous work by S. Chen [10], an analytical dislocation activation diagram (DAD) has been developed to investigate the activation conditions of full dislocation and de-correlation. The effects of several alloy parameters on the activation conditions were investigated. For both de-correlation and full dislocation looping, it was found that the activation condition is sensitive to both geometry properties and physical parameters. The geometry property is represented by precipitate microstructure and the corresponding average channel width. Physical parameters include shear modulus, lattice friction, stacking-fault energy and work hardening.

According to the work by S. Chen [10], it has been found that de-correlation and full dislocation happens at different loading condition in one alloy. Compared with de-correlation activation, full dislocation activation happens in a wider range of applied stress direction. De-correlation only happens when the threshold stress of leading Shockley partial is lower than that of trailing, which means the activations of leading and trailing partials are able to be separated by an intermediate level of applied stress.

Besides the densely distributed dislocation sources throughout crystal, in many cases, the dislocation sources are very rare or only concentrated at grain boundaries. Then, the creep deformation can be viewed as a percolation process starting from the dislocation source. In this case, average channel width no longer decides the selection of the looping mechanisms. As will be shown, local channel effect must be considered in order to
calculate the population of each mechanism (full dislocation, de-correlation, or inactivation). However, in any elementary-defect level simulation of the percolation process such as the phase field approach, consideration of local channel effect largely increases time complexity as well as memory cost. To reduce the computation cost, an alternative approach which generates similar results as phase field method but is more computationally efficiency is developed, in order to implement this model in an industrial environment.

In this work, a percolation simulation approach is designed based on the analytic DAD diagram and SEM observation of precipitate microstructure. Firstly, a local DAD is calculated which reveals critical channel width based on physical parameters such as shear modulus, stacking-fault energy and lattice friction. At the same time, SEM pictures are digitized so that channel width distribution can be recognized automatically by image processing codes. Then the local channel map is drawn by using the digitized SEM picture and critical channel width value. Finally, percolation simulation is performed based on flooding algorithm and by using the local channel map. By doing the percolation simulation, activation area of full dislocation looping and de-correlation are obtained, which works as input to other creep rate models. In order to validate the fast-acting percolation model, a phase-field simulation is performed in a select zone of the microstructure as a comparison.
5.2. **Dislocation activation diagram (DAD) of local channel width**

In the fast-acting approach, critical channel widths of full / de-correlation activations are firstly calculated by using local DAD. The local DAD actually does not use any microstructure information, but only uses a combination of physical parameters such as stacking fault, shear modulus, lattice friction and work hardening. Since critical channel width also depends on loading condition, resolved shear stress along the total Burgers vector is set in the local DAD calculation.

The critical conditions of dislocation activation are represented by boundaries in a 2-D space: stress magnitude – direction space. The critical channel width is calculated when the external loading condition exactly lays on a boundary of local DAD, which means the fulfillment of the following equations:

\[
\tau_{\text{crt}}(\text{ChW}) = \sigma_{\text{app}} \quad (33)
\]

\[
\phi_{\text{crt}}(\text{ChW}) = \theta_{\text{app}} \quad (34)
\]

Where ChW is channel width, \(\tau_{\text{crt}}\) is the magnitude of critical stress and \(\phi_{\text{crt}}\) is the direction, \(\sigma_{\text{app}}\) is the magnitude of applied stress and \(\theta_{\text{app}}\) is the direction. A solution of critical ChW is obtained, when both the equations are satisfied. The parameters follows the values in Table 5 (in Chapter 4), Table 7, Table 8 and Table 9 (in Section 5.5).

The critical channel width works as a criterion which decides whether a dislocation can locally pass through when a dislocation segment meets a local channel. Before a dislocation segment meets any narrow channel, it can pass through the matrix continuously. In the percolation simulation, a dislocation line is set to proceed from the
source on the simulation box and into a precipitate microstructure obtained by SEM. Percolation simulation will give the sheared area fraction and percolation distance. Consequently, the activation probability of each dislocation configuration can be estimated.

Figure 110. A digitalized SEM picture of the HL11 microstructure. The red color indicates the γ' particles, and the blue color means the γ matrix.

Figure 111. A DAD diagram is calculated when the average channel width (116 nm) of the above HL11 microstructure is used. The calculation shows that a full dislocation is active.
Figure 112. A deformation process is simulated by the phase-field approach when an AB dislocation interacts with the HL11 microstructure. The area of the ISF activation is obviously larger than the area of the full dislocation percolation.
Figure 113. The later stage of a deformation process is simulated by the phase-field approach when an AB dislocation interacts with the HL11 microstructure. The area of the ISF activation is obviously larger than the area of the full dislocation percolation. The δB dislocation is decoupled from the Aδ dislocation.

In Figure 110, there is a digitalized HL 11 microstructure. The average channel width is calculated to be 116 nm. Then the dislocation activation diagram is calculated, which shows that when applied stress (103Ksi) is along [100], full dislocation is active. However, the phase field simulation in Figure 112 and Figure 113 shows a large area of de-correlation, which means only leading partial percolation is active. At the same time, the full dislocation is only active in the vicinity of initial dislocation location (dislocation source at simulation box).

The critical channel width of full dislocation is analyzed according to phase field simulation. The critical channel width is decided to be 67.5nm. Use this channel width, DAD is re-calculated, where the loading condition lays exactly on the boundary between full dislocating and de-correlation zone.
Figure 114. The critical channel width, which separates the full dislocation activation and the de-correlation, is characterized by the phase-field simulation.

Figure 115. A DAD diagram is calculated when the critical channel width (67.5 nm) is used. The boundary between the full dislocation activation and the de-correlation lays on the applied stress condition. The applied stress condition is represented by the green dot which is marked by a red dashed circle.

This consistent between phase field simulation and DAD diagram with critical channel width implies that it is feasible to establish a fast-acting model which predicts the deformation mechanism population without doing phase field simulation. The critical channel width can be directly calculated by DAD, and there is no need to use phase field
simulation to check the interaction between dislocation segments and local channels. Instead, a fast-acting percolation simulation can be performed by using this critical channel width.

5.3. Local channel map

In the ME3 alloy which is shown in Figure 116, the critical channel width is calculated directly by using local DAD diagram. The loading condition is 80 Ksi along [100]. And the temperature is 1300°F. As a comparison, the DAD with the average channel width (Figure 118) is firstly calculated. Again, the average channel width predicts the activation of full dislocation throughout the crystal, which is not supported by phase field simulation.

![Image](image)

Figure 116. A digitalized ME3 microstructure. The black color indicates the γ' particles, and the white color means the γ matrix. The zone where the following calculations are performed is inside the red dashed box.
Figure 117. The local channels are displayed in the digitalized ME3 microstructure.

Figure 118. A DAD diagram is calculated when the average channel width of the ME3 is used.

**Local channel map at 80Ksi/1300°F**

The critical channel width at 80Ksi/1300°F is firstly determined by using local DAD diagrams in Figure 119 and Figure 120. The critical channels are then visualized in the channel map of Figure 121. Red channels indicate narrow channels which do not allow full dislocation to percolation but allow leading partials to pass through. Blue color indicates much narrower channels which do not allow any dislocation to pass through. Any full dislocation originated within the red colored zone cannot expand by exceeding
this zone, although average channel width predicts full dislocation activation throughout the crystal.

Figure 119. A DAD diagram is calculated when the critical channel width of the full dislocation activation is used. The temperature is 1300°F.

Figure 120. A DAD diagram is calculated when the critical channel width of the de-correlation is used. The temperature is 1300°F.
Figure 121. Narrow local channels are displayed in the digitalized ME3 microstructure. The red channels are narrower than the critical channel width of the full dislocation. The blue channels are narrower than the critical channel width of the de-correlation. The loading condition is 80Ksi/1300°F.

Local channel map at 80Ksi/1600°F

Following the same procedure in the previous section, the narrow channel map is visualized in Figure 122. Red channels do not allow full dislocation to percolation but allow leading partials to pass through. Blue color indicates much narrower channels which do not allow any dislocation to pass through. Three orange pathways are displayed which allows full dislocation to penetrate through the crystal. In this case, due to the higher temperature, lattice friction and Orowan looping strength both decrease. As a result, many channels which prohibit dislocation movement at 1300°F are now wider than the critical channel width.
Figure 122. Narrow local channels are displayed in the digitalized ME3 microstructure. The red channels are narrower than the critical channel width of the full dislocation. The blue channels are narrower than the critical channel width of the de-correlation. The loading condition is 80Ksi/1600°F. Three percolation pathways are indicated by the orange arrows.

Narrow channel maps at 60Ksi/1300°F and 60Ksi/1600°F

Following the same procedure in the previous section, in the cases of 60Ksi/1300°F and 60Ksi/1600°F, the narrow channel map is visualized in Figure 123 and Figure 124. In these cases, there is no difference between critical channels of full dislocation and de-correlation. When a channel is narrower than the critical value, both full dislocation and de-correlation cannot be active. Blue color indicates these narrow channels. When the temperature is raised to 1600°F, more channels can be passed through by dislocations. Due to the higher temperature, lattice friction, and Orowan looping strength both decrease.
Figure 123. Narrow local channels are displayed in the digitalized ME3 microstructure. The blue channels are narrower than the critical channel width. The loading condition is 60Ksi/1300°F.

Figure 124. Narrow local channels are displayed in the digitalized ME3 microstructure. The blue channels are narrower than the critical channel width. The loading condition is 60Ksi/1600°F.

5.4. Orowan looping simulation at 80Ksi/1300°F:

Based on the narrow channel map, a percolation simulation is performed by using flooding algorithm. In Figure 125, simulations show that when the dislocation sources are
concentrated at the simulation box boundaries, both percolation distance and dislocation activation area are very small.

Our calculation has been validated by TEM observations [90] on stacking fault configuration. In ME3, when tertiary volume fraction is high, de-correlation is widely observed. However, when tertiary is low, de-correlation disappear. Figure 126 is a 2-D contour of mechanism population when temperature and tertiary volume fraction varies.

![Full dislocation shearing in matrix and Partial dislocation shearing in matrix](image)

Figure 125. The percolation simulation is performed when full dislocation is initiated at the simulation box boundaries of (A) the left side, (B) the right side, (C) the lower side, and (D) the upper side. The yellow color means that the matrix has been sheared by the full dislocation, the cyan blue indicates the de-correlation area, and the dark blue means the inactivation. The γ′ particles are displayed in the red color. The percolation distance of the full dislocation is indicated by the black arrow.
5.5. Fast-acting yield strength model of 718-type superalloy

The development of fast-acting yield strength model

In this part, a fast-acting yield strength model for 718-type superalloy is developed. The model predicts the yield strength as a function of temperature and average precipitate size and volume fraction of $\gamma''$ phase. Several major strengthening mechanisms are considered in the model, including (a) precipitation hardening, (b) lattice strengthening (solid-solution hardening (SSH) + forest dislocation hardening) and (c) grain boundary strengthening (Hall-Petch relation). The temperature-dependent of physical parameters into the fast-acting model is included in this model. In this model, a linear superposition of deformation mechanisms is applied. Meanwhile, the model uses shear modulus from literature [91]. Only stacking fault energies of the $\gamma''$ phase and the cut-off particle size are the fitting parameters in this model.
The development of the fast-acting yield strength model follows 5 steps. In Step 1, detailed-level TEM characterization, *ab initio* calculations, and phase field simulations are done to determine the microstructure, generalized stacking fault (GSF) energy surface and relevant dislocation configurations. In Step 2, the data flow of the model is setup and input parameters are obtained from the information gathered in Step 1. Then, in Step 3, the total yield strength is calculated, which requires analytical expressions and numerical data of each deformation mechanism. Validation and implementation of the model are done in Step 4. A flowchart of the model development is shown in Figure 127.

According to the *ab initio* calculation of the GSF energy surface and phase field simulations carried out in previous sections, various dislocation + fault configurations have been discovered. According to the recent phase field simulations and TEM observations, the $\frac{1}{2}<112>$-type dislocation configurations have been identified as the dominating ones for the given microstructures. Then precipitation hardening equations are derived based on models developed in the literature [29]. The major advances made for these hardening equations are the consideration of stacking-fault transformation and partial dislocation generation in $\gamma''$ particle shearing processes.
The major input parameters of the fast-acting model are listed in the following Tables. The references and instructions on how to use some of the parameters are also included in the Tables. The lattice parameters, full dislocation Burgers vector, and partial dislocation Burgers vector follow the values in the $\gamma$ phase matrix.

It should be mentioned that the average particle size in the model is a 2D equivalent size. In order to use database such as PANDAT in which precipitation model is in 3D, a 3D $\rightarrow$ 2D conversion is necessary:

$$d_{avg,2D} = 0.78 \times d_{avg,3D}$$ (35)

The conversion parameter 0.78 follows the work by Ardell [92].
<table>
<thead>
<tr>
<th>Name of parameter (unit)</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice parameter of $\gamma$ phase (m)</td>
<td>$a$</td>
<td>3.60E-10 [93]</td>
</tr>
<tr>
<td>Burgers vector of full dislocation in $\gamma$ phase (m)</td>
<td>$b_f$</td>
<td>2.55E-10</td>
</tr>
<tr>
<td>Burgers vector of partial dislocation in $\gamma$ phase (m)</td>
<td>$b_p$</td>
<td>1.47E-10</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>$\nu$</td>
<td>0.313</td>
</tr>
<tr>
<td>Taylor's factor</td>
<td>$M$</td>
<td>3.06</td>
</tr>
<tr>
<td>Hall-Petch effect (Ksi)</td>
<td>$\Delta \tau_{HP}$</td>
<td>34.5 [94]</td>
</tr>
<tr>
<td>Aspect ratio of $\gamma''$</td>
<td>$\omega_{\gamma''}$</td>
<td>3.34 (obtained from phase field simulation for typical average particle size of ~41 nm)</td>
</tr>
</tbody>
</table>

Table 6. The temperature-independent model parameters

<table>
<thead>
<tr>
<th>Symbol (unit)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_{p1}$ (Pa/K$^3$)</td>
<td>6.506</td>
</tr>
<tr>
<td>$G_{p2}$ (Pa/K$^2$)</td>
<td>-2.805E4</td>
</tr>
<tr>
<td>$G_{p3}$ (Pa/K)</td>
<td>-1.233E6</td>
</tr>
<tr>
<td>$G_{p4}$ (Pa)</td>
<td>8.255E+10</td>
</tr>
<tr>
<td>Shear modulus (Pa): $G= G_{p1}*T_{K}^3 + G_{p2}*T_{K}^2 + G_{p3}*T_{K} + G_{p4}$</td>
<td>$T_K$: Temperature in K; $T_f$: Temperature in ºF; $T_K = 5/9*(T_f+460)$</td>
</tr>
</tbody>
</table>

Table 7. The model parameters related to shear modulus (temperature-dependent). [91]

| $\gamma'$ phase APB energy (J/m$^2$) | $\Gamma_{APB, \gamma'} = 0.181*(1-(T_K-485)*2.95E-4)$ |
| $\gamma''$ phase APB energy (J/m$^2$) | $\Gamma_{\gamma''} = gp_4* T_K^4 + gp_3* T_K^3 + gp_2* T_K^2 + gp_1* T_K + 0.59$ |
| $\gamma''$ phase APB-like energy (J/m$^2$) | $\Gamma_{APB-like, \gamma''} = 495/590*\Gamma_{\gamma''}$ |
| $\gamma''$ phase SISF energy (J/m$^2$) | $\Gamma_{SISF, \gamma''} = 613/590*\Gamma_{\gamma''}$ (J/m$^2$) |

Table 8. The model parameters related to stacking-fault energy (temperature-dependent).
<table>
<thead>
<tr>
<th>Symbol (unit)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sp1 (Ksi/K)</td>
<td>-0.0377</td>
</tr>
<tr>
<td>Sp2 (Ksi)</td>
<td>39.15</td>
</tr>
<tr>
<td>Lattice stress (Ksi)</td>
<td>$\Delta \tau_{LS} = Sp1 \cdot T_K + Sp2$</td>
</tr>
<tr>
<td>$T_K$: Temperature in K; $T_f$: Temperature in °F; $T_K = \frac{5}{9}(T_f + 460)$</td>
<td></td>
</tr>
</tbody>
</table>

Table 9. The model parameters related to lattice stress (solid solution hardening + forest dislocation hardening, temperature-dependent). [27]

While the average particle sizes and volume fractions are obtained from the PANDAT software, particle size distribution is obtained either by phase field simulations of precipitation in IN718 [82] (an example can be found in), or approximated by log-normal distributions. The phase field simulations reveal a bimodal distribution, and the cut-off particle size (the largest particle size in the distribution) is determined to be approximately 80nm.

Figure 128: The particle size distribution obtained from the phase-field simulations.
An analytical expression for the log-normal distribution is tuned when the average particle size and cut-off particle size are known from phase field simulation. For example, the unimodal log-normal type particle size distribution is given by the following equations:

\[
f(d_{y,l}) = \frac{1}{d_{y,l} \times 1E9 \times \sigma \sqrt{2\pi}} e^{-\frac{(\ln(d_{y,l} \times 1E9) - \mu)^2}{2\sigma^2}}
\]  

(36)

where

\[
\mu = \ln \left( \frac{d_{avg,y}}{1 + \frac{\nu}{d_{avg,y}}} \right)
\]  

(37)

\[
\sigma = \sqrt{\ln \left( 1 + \frac{\nu}{d_{avg,y}^2} \right)}
\]  

(38)

\(d_{y,l}\) is the individual particle size, \(d_{avg,y}\) is the average particle size and \(\nu\) is the cut-off particle size.

Typical examples of the log-normal precipitate size distribution are shown in **Figure 129**. The cut-off particle size in these plots is set to be 80 nm, which is obtained from phase field simulations.
Figure 129: The typical examples of a unimodal log-normal particle size distribution when the cut-off particle size is chosen to be 80 nm.

Besides the particle size distribution, the phase field simulations also provide the aspect ratio of \( \gamma'' \) particles required in the fast-acting yield strength model [82]. Note that in the experiment the aspect ratio of \( \gamma'' \) particles is estimated from the composite particles while in phase field simulation the aspect ratio of individual \( \gamma'' \) particles is calculated.

In order to calculate the critical particle size, the average channel width (\( C_{h_{\gamma''}} \)) between \( \gamma'' \) precipitates needs to be determined. Again, this parameter can be determined either from phase field simulations or from an analytic expression. When determined by the phase field simulations, an example of such a calculation is illustrated in Figure 130. The results from the phase field simulations are used to validate the following analytic expression which will be used in the fast-acting model:

\[
C_{h_{\gamma''}} = \omega_{\gamma''}^{-\frac{1}{3}} \left( \frac{2 + \omega_{\gamma''}^{-1}}{3} \right)^{-\frac{1}{4}} L_s
\]

(39)
\[ L_s = \frac{1.0746}{\sqrt{f' \left( \frac{d_{avg,y''}}{2} \right)^2}} - d_{avg,y''} \]  

The comparison between the phase field simulation and the analytic expression is given in Table 10.

![Image](image1.png)

(a)                                   (b)

Figure 130: The channel widths among the \( \gamma'' \) particles (the blue lines in (b)) identified for the precipitate microstructure shown in (a) generated by the phase field simulations.

<table>
<thead>
<tr>
<th>Method</th>
<th>Average channel width (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Determined from phase field simulations</td>
<td>20.86</td>
</tr>
<tr>
<td>Calculated by the analytic expression</td>
<td>19.96</td>
</tr>
</tbody>
</table>

Table 10. The comparison of average channel width between \( \gamma'' \) particles determined from the precipitate microstructures generated by the phase field simulations and calculated from the analytic expression.
**Dominating dislocation configuration**

In Chapter 3, DFT-based phase field simulations have revealed that the <112> type dislocations are easily activated in IN718, which has been confirmed by the concurrent TEM observations [30]. More importantly, various APB-like stacking fault or SISF SF ribbon configurations have been discovered by the phase field simulations, which constitute the dominant shearing mechanisms of the γʺ precipitates in IN718 and define the precipitation hardening mechanisms of the alloy.

In order to describe properly the stacking fault ribbon strengthening, the following general form of shearing-strengthening is used in the fast-acting model:

\[
\Delta \tau_s(\theta) = \Delta \tau_{SFC}(\theta) - \Delta \tau_{SFA}(\theta) + \Delta \tau_{RP}(\theta) + \Delta \tau_{frict}(\theta)
\]  

(41)

where \( \theta \) is the angle between the applied shear stress and Burgers vector. \( \Delta \tau_s \) is the critical shear stress resolved on \{111\} glide plane, \( \Delta \tau_{SFC}(\theta) \) is from stacking fault creation and \( \Delta \tau_{SFA}(\theta) \) is the strength reduction when stacking fault annihilation happens.

If stacking fault creation and annihilation take place simultaneously during the shearing process, a stacking fault ribbon is created. \( \Delta \tau_{RP}(\theta) \) is the looping strength of partial dislocation created by stacking fault transformation and \( \Delta \tau_{frict}(\theta) \) is lattice friction including SSH and dislocation-forest hardening. The contributions of \( \Delta \tau_{RP}(\theta) \) and \( \Delta \tau_{frict}(\theta) \) are relatively small as compared to those from the two leading terms in Eq. (2).

When AC+AB dislocation is active, the stacking fault ribbon and related Burgers vector for each variant of γʺ are listed in Table 11.
Table 11: The stacking fault ribbon and the related Burgers vector for each variant of \( \gamma'' \)

<table>
<thead>
<tr>
<th>Variant</th>
<th>SF creation</th>
<th>SF annihilation</th>
<th>Burgers vector related with SF creation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1\textsuperscript{st}</td>
<td>SISF</td>
<td>-SISF</td>
<td>CA</td>
</tr>
<tr>
<td>2\textsuperscript{nd}</td>
<td>SISF</td>
<td>-SISF</td>
<td>BA</td>
</tr>
<tr>
<td>3\textsuperscript{rd}</td>
<td>APB-like</td>
<td>-APB-like</td>
<td>CA</td>
</tr>
</tbody>
</table>

**Framework of the fast-acting yield strength model**

The overall framework of the fast-acting yield strength model consists of four essential parts a) microstructure characterization, b) shearing vs. looping population prediction, c) superposition of each mechanism and d) parameter fitting and model validation.

In the first part of the model, the major microstructural parameters such as average particle size and volume fraction are obtained from PANDAT software. The particle size distribution is assumed to be log-normal and its cut-off particle size is one of the fitting parameters. The aspect ratio of \( \gamma'' \) particles is important for predicting shearing vs. looping population and is obtained from phase field simulations.

In the second part of the model, populations of sheared vs. looped particles are calculated as an intermediate output. These calculations require detailed microstructural inputs from part 1. The population is actually a weighting factor of different hardening mechanisms. These mechanisms include shearing and looping of each variant of \( \gamma'' \) phase.

In the third part of the model, the yield strength increment from precipitation hardening is first calculated. This part uses inputs from both the 1\textsuperscript{st} and 2\textsuperscript{nd} parts. Then contributions from all strengthening mechanisms including lattice stress hardening (SSH + forest...
dislocation) and grain boundary strengthening (Hall-Petch) are added, and the total yield strength of the alloy is predicted as a function of temperature.

Figure 131. The overall framework of the fast-acting yield strength model

**Shearing vs. looping population calculation**

With a given particle size distribution and calculated critical particle size, populations of shearing vs looping can be determined (**Figure 132**) and serve as inputs to the yield strength model. The alloy’s yield strength depends sensitively on these populations. Whether a precipitate is sheared or looped will depend on microstructural characteristics such as particle size, volume fraction, shape (aspect ratio) and inter-particle distance (i.e., channel width). Thus, detailed heat-treatment conditions control these populations. In
addition, the shearing vs. looping population is also controlled by service temperatures, since the line-tension of dislocations and SF energy in the sheared particles depend on the service temperature.

![Image](image.png)

Figure 132. The meanings of the mechanism population and the critical particle size in a given particle size distribution.

The aspect ratios of the $\gamma'$ and $\gamma''$ precipitates are assumed constant and inter-particle distance is assumed to be uniform. Note that these are rough approximations because, as mentioned above, the aspect ratio is a function of particle size, and the spatial distribution of precipitates may deviate significantly from uniform.

The critical size for the transition from shearing to looping for individual precipitates can be determined by making the shearing stress equals to the looping stress given by the following equations [29]:

$$s\tau_{s,\gamma',k}(d_{c,\gamma',k}) = \tau_{L,\gamma'',k}$$

(42)

where
In these equations, \( k \) indicates the \( k \)-th variant of \( \gamma'' \) precipitates. \( \tau_{s,Y''} \) and \( \tau_{L,Y''} \) are the critical stresses of shearing and looping, respectively. \( d_{c,Y''} \) is the individual particle size. The critical stress of looping consists of three parts: line-tension (\( \tau_{LT,Y''} \)), friction force from \( \gamma' \) particles in channels (\( \tau_{Y',chl} \)) and other obstacles (lattice fraction, forest dislocations, etc.). \( C_{h,Y''} \) is the average channel width between \( \gamma'' \) precipitates, and \( f_{\gamma'} \) and \( f_{\gamma''} \) are the volume fractions of \( \gamma' \) and \( \gamma'' \) phases, respectively.

The analytical equations used for calculating the critical particle size for the shearing–looping transition are:

\[
d_{c,Y'',1} = \sqrt{\frac{2f_{\gamma'}/\phi_1}{\langle 1 + \nu - 3\nu\sin^2\gamma \rangle}} \left( \frac{\phi_1 \tau_{LT,Y''} + f_{\gamma''} \Gamma_{SISF,Y''}}{0.72 + f_{SISF,Y''}} \right)^2
\]  

(51)
\[ d_{c,y''} = d_{c,y''} \]
\[ d_{c,y''} = \frac{\sqrt{a_{y''} g b f^2}}{2f_{y''}} \left( \frac{\phi_3 T_{y''} + f_{y''} \gamma_{APBlike,y''}}{0.72 \cdot \gamma_{APBlike,y''}^{1.5}} \right)^2 \]

When the critical particle size and the particle size distribution are determined, the populations of precipitates sheared vs looped can be calculated using the following equations:

\[ W_{k,1} = \frac{\sum_{d_{y''} < d_{c,y''}} f_k(d_{y''})}{\sum_{d_{y''} \neq d_{c,y''}} f(d_{y''})}, \quad k = 1, 2, 3 \]  

\[ f_k(d_{y''}) = \frac{1}{3} f(d_{y''}) \]  

\[ W_{k,1} = 1 - W_{k,2} \]

where \( W_{k,1}, W_{k,2} \) are the weighting factors of the shearing and looping mechanisms in the \( k \)-th variant, respectively. Equation (16) assumes that all three variants of \( y'' \) particles have identical size distribution. The meanings of each \( W_{k,i} \) and the corresponding strengthening, \( \Delta \tau_{k,i} \), are listed in Table 12.

<table>
<thead>
<tr>
<th>Variant</th>
<th>Shearing population</th>
<th>Shearing strength</th>
<th>Looping population</th>
<th>Looping strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variant 1</td>
<td>( W_{1,1} )</td>
<td>( \Delta \tau_{1,1} )</td>
<td>( W_{1,2} )</td>
<td>( \Delta \tau_{1,2} )</td>
</tr>
<tr>
<td>Variant 2</td>
<td>( W_{2,1} )</td>
<td>( \Delta \tau_{2,1} )</td>
<td>( W_{2,2} )</td>
<td>( \Delta \tau_{2,2} )</td>
</tr>
<tr>
<td>Variant 3</td>
<td>( W_{3,1} )</td>
<td>( \Delta \tau_{3,1} )</td>
<td>( W_{3,2} )</td>
<td>( \Delta \tau_{3,2} )</td>
</tr>
</tbody>
</table>

Table 12. The \( y'' \) phase strengthening mechanisms list
**Total yield strengthen calculation**

For IN718, the total yield strength ($\tau_y$) consists of contributions from precipitation hardening ($\Delta \tau_{pp}$), lattice strengthening ($\Delta \tau_{LS}$) (SSH + forest dislocation) and grain boundary strengthening (i.e., the Hall-Petch effect) ($\Delta \tau_{HP}$), which are added together linearly in the fast-acting model.

![Diagram of the model](image)

**Figure 133. The structure of the fast-acting yield strength model**

Since there are three different variants of $\gamma''$, even only one dislocation configuration (e.g., a single AB+AC dislocation) is considered, there are still several deformation modes, as summarized in Table 13. In this model, strengthening effects of ABP-like ribbon and SISF ribbon are both calculated by using modified expressions based on APB ribbon shearing.

194
<table>
<thead>
<tr>
<th>Variant</th>
<th>Shearing mechanisms</th>
<th>Looping mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>SISF ribbon shearing</td>
<td>Full dislocation looping</td>
</tr>
<tr>
<td>2nd</td>
<td>SISF ribbon shearing</td>
<td>Full dislocation looping</td>
</tr>
<tr>
<td>3rd</td>
<td>APB-like ribbon shearing</td>
<td>Full dislocation looping</td>
</tr>
</tbody>
</table>

Table 13: The deformation mechanisms in the $\gamma''$ particles when a AC+AB ($\frac{1}{2} <112>$) dislocation is considered

When the three variants have the same population, the weighting factors for their contributions to the strength are $W_{k,1}$ and $W_{k,2}$, and $\sum_{i=1,2,3}(W_{k,1} + W_{k,2}) = 1$, where $k$ represents the k-th variant, and “1” for shearing and “2” for looping. Then the yield strength increment by precipitation hardening can be calculated by the following equations [29] [92, 95-98]:

$$\Delta \tau_{pp} = M[\Delta \tau'_y, s + 2 * \sum_{j=1,2}W_{1,j} \Delta \tau_{1,j} + W_{3,1} \Delta \tau_{3,1} + W_{3,2} \Delta \tau_{1,2}]$$  \hspace{1cm} (57)

$$\Delta \tau'_{y,s} = \frac{1}{\phi_3} f_y' \Gamma_{APB,y'}$$  \hspace{1cm} (58)

$$\Delta \tau_{1,1} = \frac{1}{\phi_1} \left( \frac{\Gamma_{SISF,y}^{1.5}}{\sqrt{\alpha _y^* G b_f^*}^2} \ast \frac{2d_{avg,y} f_y^*}{\alpha ^* G b_f^*} \ast 0.72 - f_y^* \ast \Gamma_{SISF,y}^* \right)$$  \hspace{1cm} (59)

$$\Delta \tau_{2,1} = \Delta \tau_{1,1}$$  \hspace{1cm} (60)

$$\Delta \tau_{3,1} = \frac{1}{\phi_3} \left( \frac{\Gamma_{APBlike,y}^{1.5}}{\sqrt{\alpha _y^* G b_f^*}^2} \ast \frac{2d_{avg,y} f_y^*}{\alpha ^* G b_f^*} \ast 0.72 - f_y^* \ast \Gamma_{APBlike,y}^* \right)$$  \hspace{1cm} (61)

$$\Delta \tau_{1,2} = \frac{2 b_f}{\phi_3} \frac{G b_f}{2 \pi c h_y} \frac{1}{1-n} \left( \frac{1+3v \sin^2 75^\circ}{1-v} \right) \ln \left( \frac{c h_y}{b_f} \right)$$  \hspace{1cm} (62)

$$\Delta \tau_{3,2} = \Delta \tau_{2,2} = \Delta \tau_{1,2}$$  \hspace{1cm} (63)
\[ \phi_1 = 1.7321 \times b_f + 0.5 \times f_{\gamma'} \times b_p \]  
\[ \phi_3 = 1.7321 \times b_f \]  

where \( \Delta \tau_{pp} \) is the yield strength increment due to precipitation hardening in a polycrystalline alloy. It is calculated from the single crystalline strength and the Taylor's factor \( M \). \( \Delta \tau_{\gamma'p} \) represents contributions from \( \gamma' \) particles, and \( \Delta \tau_{k,1} \) and \( \Delta \tau_{k,2} \) represent the shearing and looping strengthening of the \( k \)-th variant of \( \gamma'' \) particles, respectively. The total yield strength is then given by:

\[ \tau_y = \Delta \tau_{pp} + f_{\gamma} \Delta \tau_{LS} + \Delta \tau_{HP} \]  

**Model calibration and validation**

There are still several model parameters that are not available in literature or experiments. These parameters are determined by fitting the model predictions to the experimental measurements of yield strength as a function of temperature. Some of these parameters (gp1, gp2, gp3, gp4) are related to the temperature dependence of \( \gamma'' \) phase stacking-fault energy. Another fitting parameter is the cut-off size of the log-normal distribution.
Figure 134: The comparison between the model prediction and the experimental measurement of the yield strength of IN718 as a function of the temperature.

A comparison between the predicted and experimentally measured yield strength as function of temperature is shown in Figure 134, where a log-normal particle size distribution is used in the fast-acting model.

**Model predictions**

The most important intermediate outputs are critical particle size, strength increment and population of each mechanism. The critical particle size is plotted in Figure 135 as a function of average particle size and service temperature. When the average particle size increases for a fixed volume fraction, the average channel width increases dramatically. As a consequence, more particles will be looped and the critical particle size becomes smaller. When the service temperature increases, the critical stress of looping drops faster than that of shearing and. Again, the critical particle size becomes smaller.
The populations of particle sheared vs looped and their contributions to the strength are also plotted as functions of the average particle size and service temperature in Figure 136, respectively.

Figure 135: The critical particle size as a function of the average particle size and the service temperature.

Figure 136: The population of each deformation mechanism as a function of the average particle size and the service temperature.
Figure 137: The strength of each deformation mechanism as a function of the average particle size and the service temperature.

Figure 138: The total yield strength as a function of the average particle size.

Note that when the average particle size is smaller the shearing mechanism is dominating and when the average particle size becomes larger, the looping mechanism controls the yield strength. As a result, the total yield strength shows a peak in the vicinity of $\gamma''$ average particle size of 30 nm, as shown in Figure 137.
The final output of the model is the yield strength. The log-normal particle size distribution shown in Figure 132 is used in this calculation. The yield strength is predicted as a function of precipitate volume fraction, average particle size and temperature, which is shown in Figure 138 and Figure 139.

![Figure 139](image)

Figure 139: The prediction of the yield strength as a function of the total volume fraction of the precipitates, and the average particle size at the room temperature. A log-normal particle size distribution is used in this calculation.

At both room temperature and 1000°F, the total yield strength reaches the maximum when the average particle size is ~30 nm. The peak indicates a transition from shearing dominated deformation to looping dominated deformation.

5.6. Summary

(1) The fast-acting Orowan looping model was developed for Ni-based superalloys with γ/γ' microstructure. The simulation results of the model imply that, when the dislocation sources are rare throughout the crystal, the percolation distance of full dislocation is very
small. In the vicinity of the dislocation source, a closed zone that constrains the
movement of full dislocation is formed by the narrow channels. By using the critical
width of the channel as a selection criterion, the narrow channels are identified from the
local channel map. The critical width of the channel was calculated by using the
dislocation-activation-diagram (DAD), which was originally designed to investigate the
effect of the average width of the channel. The critical width of the channel is a
parameter that is independent of the specific microstructure. Instead, it is only controlled
by physical parameters, such as shear modulus, stacking-fault energy, and lattice friction.

(2) The fast-acting, yield-strength model was established for IN718. The analytical
expressions were modified to account for stacking-fault ribbon strengthening in the $\gamma''$
phase. Linear superposition of different strengthening mechanisms was used in the total
yield strength model. The model’s major output is the yield strength, which is a function
of temperature, average particle size, and volume fraction of precipitates. However,
several intermediate outputs are displayed explicitly, including critical individual particle
size for the shearing-looping transition, shearing vs. looping particle populations, and
strength increment from each deformation mechanism.

(3) Most of the model’s parameters were calibrated against available experimental
measurements in the literature and in phase field simulations. Several parameters were
determined by fitting the model’s predictions of the alloy yield strength to the
experimentally-measured values at different temperatures. These parameters were related

201
to the temperature dependence of the $\gamma''$ phase stacking-fault energy and the cut-off size of the log-normal distribution.

(4) In the fast-acting yield strength model, $\gamma'$ and $\gamma''$ particles are assumed to be in the form of individual particles, and the three variants of the $\gamma''$ precipitates were assumed to have identical size distributions. The AC+AB (1/2<112>) dislocation configuration was assumed to be the dominant dislocation configuration. The coherency misfit stress of precipitates was ignored in this model. In addition, $\gamma'$ particles were assumed always to be sheared, which is a reasonable assumption according to both experimental observations and phase-field simulations.
Chapter 6: Summary and Future Work

6.1. Summary

In this work, the relationship between precipitate hardening effects and atomic scale process was determined through a multi-scale modeling approach. This relationship was used to explain the experimental observations in deformed superalloys and to develop an advanced yield-strength model and a creep model. The effects of precipitate stacking-fault, dislocation configuration, precipitate microstructure, and elastic misfit energy were investigated systematically, and an extensive variety of shearing and looping mechanisms were discovered. The creep mechanism population and yield strength of superalloys were quantitatively predicted by the fast-acting version of the models. Several recent experimental observations of plastic deformations of superalloys were well explained by using DFT calculation and phase field simulation. Some important outcomes of this multi-scale model can be summarized as follows:

(I) For the first time, the complete generalized-stacking-fault (GSF) potential surface of $\gamma''$ was calculated by using the DFT method. Several stacking faults in the $\gamma''$ phase were found to be unstable according to the accurate \textit{ab initio} calculation. These unstable stacking faults, once created, transformed into nearby stable structures. The stacking-fault transformation was accompanied by dislocation emissions. As a result, novel dislocation
sources were predicted in the $\gamma''$ phase-dominant superalloys. This GSF surface was used in phase-field simulation to predict the interaction between several dislocation configurations and the $\gamma''$ phase particles.

(II) The deformation mechanisms of 718-type superalloy were investigated by using the DFT-based phase-field approach. The $<112>$-type dislocations were found to be dominant in the deformed microstructure since the emitted $<112>$-type dislocations were pinned by both $\gamma'$ and $\gamma''$ particles. Meanwhile, it was easy for the AC+AB dislocation to be active, and it was used as an input of the fast-acting, yield-strength model. Unlike the predictions of the APB-type yield-strength models in literature, ISF was predicted to be the dominant debris structure as well as having a perfect stacking sequence. The results of this work explained the recent experimental observations that APB was absent and $<112>$-type dislocations were dominant.

(III) DFT-based phase-field simulation was performed to investigate the stacking-fault formation in superalloys with $\gamma/\gamma'$ microstructure. A large amount of SISF was found in the Co-based superalloy due to the balance between stacking-fault energy and elastic energy. In the Ni-based superalloy, APB energy was too high, and only Orowan looping occurred. However, in the CoNi-based superalloy, APB energy was relatively low, and APB was left as the debris of the deformation. A stable coexistence of SISF and APB was found in the (111) triangular cross section of the Co-based superalloy. The stacking-fault energy, elastic misfit energy, and cross section morphology controlled this coexistence of weak and strong stacking-fault configurations.
(IV) The local narrow channels were found to control the Orowan looping process when the dislocation sources were rare in the crystal or they were concentrated in the vicinity of the grain boundaries. The fast-acting Orowan looping model was used to predict the volume fraction of the sheared matrix and the population of the dislocation configurations.

(V) A fast-acting, yield-strength model was developed for 718-type superalloy. Phase-field simulations were performed to calibrate the dislocation core structure and the stacking-fault configuration. The effects of temperature, particle volume fraction, and particle size distribution were considered in the model. The model was trained by using available yield-strength data from GE aviation.

6.2. Future Work

(I) In the fast-acting model, contributions to the yield strength included precipitation hardening, SSH, and the Hall-Petch effect, but misfit stress hardening was ignored. However, coherency stress fields of the $\gamma''$ precipitates could have some significant effects on the strength. For example, the $\frac{1}{2}<112>$-type dislocation configuration may not be equivalent to the three different $\gamma''$ variants, as was shown in Chapter 3.

(II) More importantly, this model assumes that all $\gamma'$ and $\gamma''$ precipitates are individual particles. However, according to recent TEM observations, $\gamma'/\gamma''$ composite particles are actually dominant in both IN718 and DA718 alloys. This composite particle morphology could alter the inter-particle spacing, misfit stress field, and shearing pathways. In this work, we did not investigate how the composite morphology influences the dominant
dislocation configurations. The impact of composite particles on the fast-acting, yield-strength model should be investigated carefully in the future.

(III) In the \textit{ab initio} calculation of GSF surface, the composition of the $\gamma''$ phase was assumed to be Ni$_3$Nb. However, in a realistic $\gamma''$ phase, multiple elements occupy the A sites and the B sites of the body-centered-tetragonal $\text{A}_3\text{B}$ structure. Especially on the B sites, significant amounts of Al exists, and the $\gamma''$ phase composition should be approximated by Ni$_3$(Nb, Al). In order to calculate the GSF surface of Ni$_3$(Nb, Al), there must be a statistical ensemble that consists of each possible atomic configuration. However, this statistical ensemble would dramatically increase the computational complexity. One technique to reduce the computational complexity is to know the most popular atomic configurations from experimental measurements, such as energy-dispersive X-ray spectroscopy (EDS).

(IV) According to the DFT calculation in this work, the ultra-low ISF energy in the $\gamma''$ phase implies the easy formation of the microtwin. A multi-layer GSF surface is able to estimate the activation energy of the microtwin. This quantitative result can be used as one of the input parameters of the crystal plasticity model, which can be used to evaluate the formation rate as well as the moving rate of the microtwin.

(V) According to the phase field simulation in Figure 22, during the deformation of Variant 1 $\gamma''$ particle by AC+AB, the pathway was changed from $\delta C \rightarrow \text{A}\delta \rightarrow \delta B \rightarrow \text{A}\delta$ (in matrix) to $\delta B \rightarrow \text{A}\delta \rightarrow \delta C \rightarrow \text{A}\delta$ (inside the particle). The atomic-scale explanation of this
change can be provided by molecular approaches, such as molecular dynamics, which are in progress.

(VI) The phase field simulation in Figure 33 displays a pattern that consists of “super particles” built up by three variants of the γ” particles. Different variants of the γ” particles tend to stay together, by which the total elastic energy is reduced. These “super particles” contribute to Orowan looping at low temperatures, since the effective particle size in the microstructure is increased by these particle clusters. The misfit stress is believed to control the formation of these “super particles,” and it is important to investigate the realistic microstructures with different levels of misfit stress. Since the misfit stress can be controlled by some parameters, such composition, a physics-based model can be developed to understand how the particle-cluster hardening effect is controlled by the method used to process the materials.

(VII) The fast-acting creep model in Figure 116 uses a digitized microstructure. It is critical to know whether the microstructure can properly represent the realistic crystal. A feasible approach is to obtain the characteristics of a representative microstructure, and, then, the “abnormal” microstructures automatically can be abandoned. In Figure 140, a framework of detection of the representative microstructure is provided.
A collection of microstructure pictures

These microstructure can be obtained by:
• Individual measurements
• Randomized sampling from a big picture

Calculate quantitative features of each picture: particle size, volume fraction, channel width, and so on.

Statistical analysis:
• Decide the characteristics of representative microstructures (inlier) and abnormal microstructures (outlier)

Figure 140: A framework of the statistical analysis of the representative microstructure.
Bibliography

[34] Zhou N. Acta Materialia, to be published.
[70] Vitek V. Crystal Lattice Defects 1974;5:1.