

CRANFIELD UNIVERSITY

Shahram Dindarlou

Modeling of Overloads in Cyclic Loading

School of Aerospace, Transport and Manufacturing
PhD in Manufacturing

PhD
Academic Year: 2021-2022

Supervisor: Dr Gustavo M. Castelluccio
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Abstract

While researchers have tried to predict mechanical response in cyclic loading, the modelling of overloads (monotonic loads among cycles) is still missing in the literature. This work presents a new crystal plasticity approach to predict the overload response.

Even though crystal plasticity models have been available for decades, quantification of material parameters is still a matter of debate. Polycrystalline experimental results can normally be reproduced by multiple sets of parameters, raising concerns about the best parameterization to predict the grain-level response. Crystal plasticity parameters has been optimised by not only fitting experimental stress-strain curves but also independent prediction of mesoscale structures in this work. We employ a unique set of parameters with limited uncertainty to reproduce the mechanical response of FCC single- and polycrystals in monotonic loading. We demonstrate that mesoscale parameters are material-invariant and can be used to model FCC metals with similar dislocation substructures such as for Cu, Ni and Al. Furthermore, the model is validated by comparing to experimental single- and poly-crystalline stress-strain curves and mesoscale dislocation substructure images.

This work also innovates with a new optimization method to calibrate the proposed crystal plasticity model parameters. We estimated model parameters for Cu, Ni, and Al and showed that these parameters are applicable to predict stainless steel response without single crystal data.

Finally, we used the model with optimised parameters to predict the overload response for Cu and NiCr alloy. The agreement with experiments for not only macroscopic response, but also mesoscale structures attributes shows robust prediction power of this

work.

Keywords

Dislocation substructures; Crystal plasticity; Mesoscale material-invariant parameterization; Single crystals, Parameter optimisation, Overload model.

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Chapter 1

Introduction

1.1 Motivation

Application of low but periodic loads can lead to metal fatigue, which is a major cause of parts failures across industries [4]. Cyclic deformation usually occurs along with monotonic overloads in service conditions, as shown in Figure 1.1. Considerable effects of the monotonic overloads on the subsequent cyclic deformation, [30, 32–34, 52, 53], require a mechanistic understanding to do inclusive fatigue failure analysis, increase safety and enable the reuse of components.

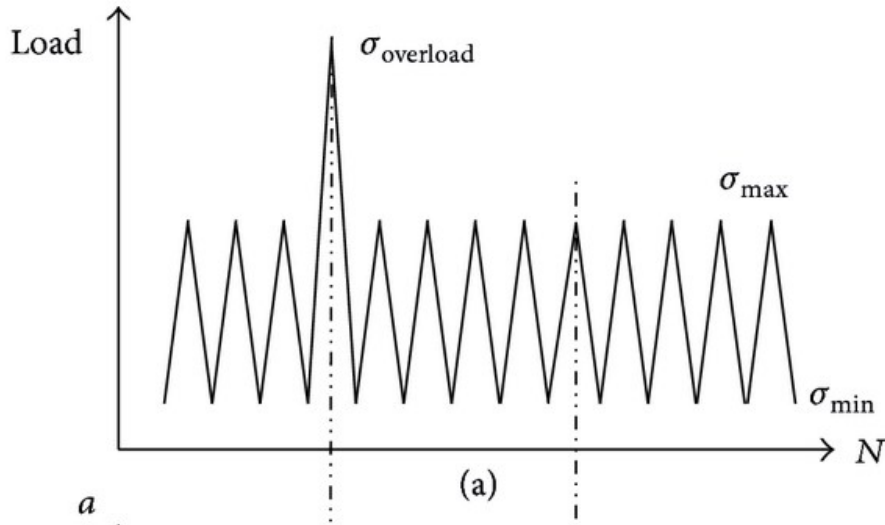


Figure 1.1: Overloads in cyclic loading

Overloads effects on the subsequent cyclic deformation have been analyzed in several experimental works, [32–34, 52, 53]. The experiment from one case (material, loading, etc.) is not usually predictive for others, and more comprehensive analysis demands predictive modelling frameworks.

Various models [54–60] have predicted fatigue crack growth rate after overloads. Both crack initiation and growth are consequences of the cyclic deformation, [4]. Lack of models to predict the effects of overloads on the subsequent cyclic deformation is the main research gap (novelty) of this work.

1.2 Modelling Strategy

Some researchers [30, 32–34, 54–60] have related macroscopic responses (stress, crack growth rate, etc.) of overloads to changes of mesoscale dislocation substructures. Dislocation substructures after overloads in the literature are equiaxed and elongated cells. The equiaxed and elongated cells are also reported, [1, 10, 11, 61], as a common structure in monotonic loading (Figure 1.2). Also, monotonic loads are similar to overloads with respect to loading time and history effect (both monotonic and overloads are being applied in one cycle). Similarities of macroscopic load applying and mesoscale dislocation substructures, make it necessary to develop a model for monotonic and use that for overloads. Linkage between macroscopic behaviour and mesoscale substructures requires a multi-scale model to include both scales.

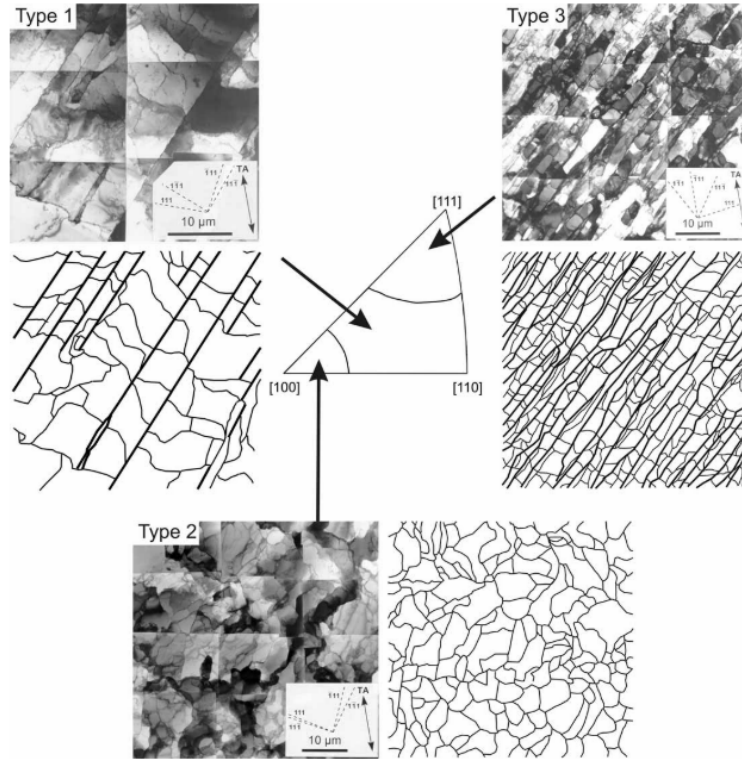


Figure 1.2: Equiaxed and elongated cells as a common structure in monotonic loading. The figure from Ref. [1].

Crystal plasticity is a powerful multi-scale modelling framework to link the macroscopic behaviour to the mesoscale substructures, [62–66] which relate to the macroscopic

behaviour by several parameters. Optimization of mentioned parameters is a key aspect for a robust linkage between macro and meso-scale and prediction power of the model.

1.3 Objectives and Outline of the Thesis

First objective of this study is to achieve a comprehensive understanding of linkages between multiples scale behaviours of materials. The physical reasons of macroscopic mechanical response of materials are discussed in Chapter 2 and the crystal plasticity tool to incorporate those multiscale interactions is described in Chapter 3.

Overloads are monotonic loads between cycles with identical substructures. Thus, **second objective** is to develop a substructure-sensitive crystal plasticity model to predict macro and meso-scale behaviours of FCC metals under monotonic loading which is explained in Chapter 4.

Parameters estimation is the main challenge and key aspect of crystal plasticity models. Hence, **third objective** is to design a new physical based crystal plasticity parameters optimisation to estimate the proposed models parameters. Details of optimisation strategy are described in Chapter 5.

Fourth objective is to integrate the proposed monotonic model with optimised parameters and cyclic model to predict overload response in cyclic loading. The integrated model is discussed in Chapter 6. Finally, implications of overall work are being discussed in Chapter 7, and conclusion and future works are summarised in Chapter 8.

Chapter 2

Multiscale Mechanistic Analysis of Experimental Data

2.1 Plastic Deformation

Heterogenous deformation of metals (Figure 2.1a) shows that plastic deformation is anisotropic and occurs in specific planes (Figure 2.1b). To understand the plastic deformation mechanism in deformed planes of crystals, an atomic structure analysis is required.

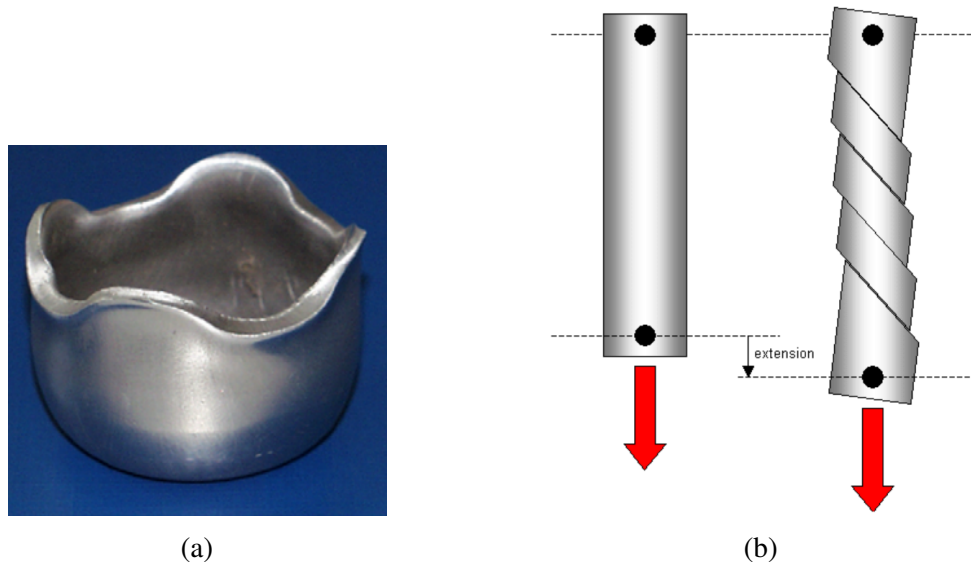


Figure 2.1: a) Heterogenous deformation of metals showed that plastic deformation is anisotropic. b) The plastic deformation in crystals under tensile loading occurs in specific planes. The figure from Ref. [2].

2.2 Crystal Atomic Structure

Atoms within metallic crystals are located in repeating patterns over a long range. Minimum repeating pattern is called a unit cell (atoms are assumed as solid hard balls). Crystalline structure with atoms situated at each corner of the unit cell and centers of all surfaces is called a face-centered cubic crystalline structure (FCC) as shown in Figure 2.2. Copper, aluminum, nickel, and 316 stainless steel has FCC crystalline structure. Similarly, crystalline structure with atoms on each corner and one at the center of the unit cell is called body-centered cubic crystalline structure (BCC) which has been seen in some metals like iron. Metals atomic structure explains the plastic deformation mechanism, [3].

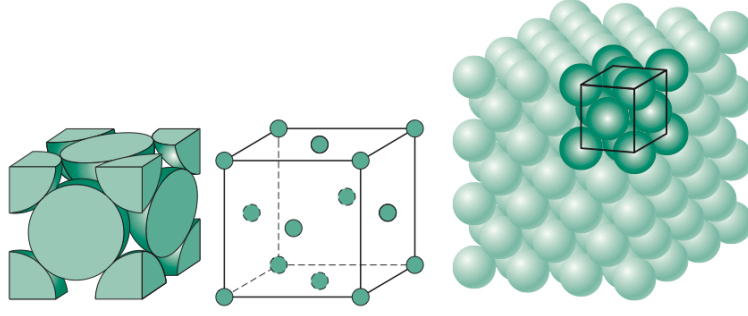


Figure 2.2: The FCC atomic structure. The figure from Ref. [3].

2.3 Plastic Deformation Mechanism

Deformed planes of single crystals (Figure 2.1b) are those with maximum atomic density, Figure 2.3. High atomic density produces repulsive force with upper and lower planes which enables the deformed plane to glide (slip) easier (compared to other atomic planes), [4]. Slip planes move along specific directions (slip directions). Combination of slip planes and directions form slip systems (Figure 2.3). The slip of atomic planes through slip systems due to applied loads results in plastic deformation, [4].

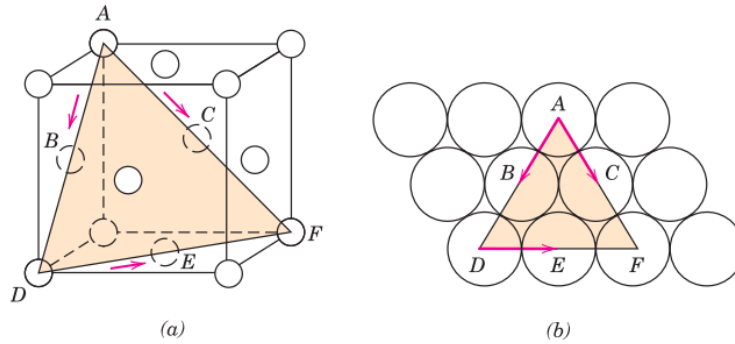


Figure 2.3: Slip planes and directions (slip systems) in FCC metals. The figure from Ref. [3].

Decomposition of applied normal stress (Figure 2.4) defines shear stress on the slip systems as (Schmid law, [4]),

$$\tau_r = \sigma(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) \quad (2.1)$$

where $\mathbf{s}^\alpha$ and $\mathbf{m}^\alpha$ correspond to the slip direction and slip plane normal of slip system α , respectively. In absence of twinning in FCC metals (high stacking fault energy metals such as copper, nickel, aluminum, etc.), slip is predominant plastic deformation mechanism. However, theoretical stress required for the movement of a defectless slip plane is very high which does not justify the plastic deformation, [4]. Hence, dislocations are introduced as a mechanism of slip plane movement (Figure 2.5).

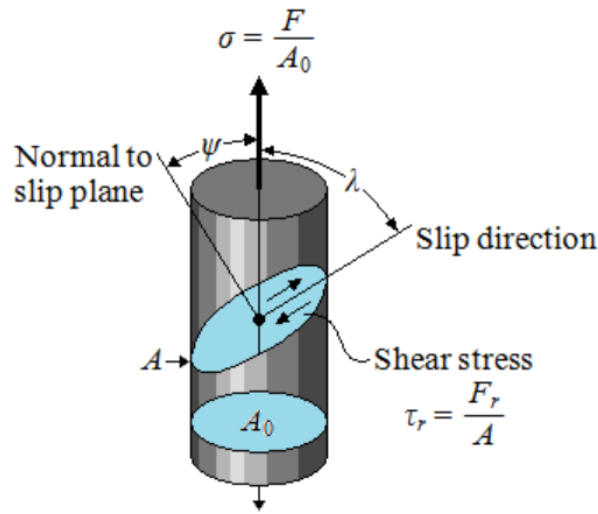


Figure 2.4: Shear stress on slip systems (Schmid law, [4]).

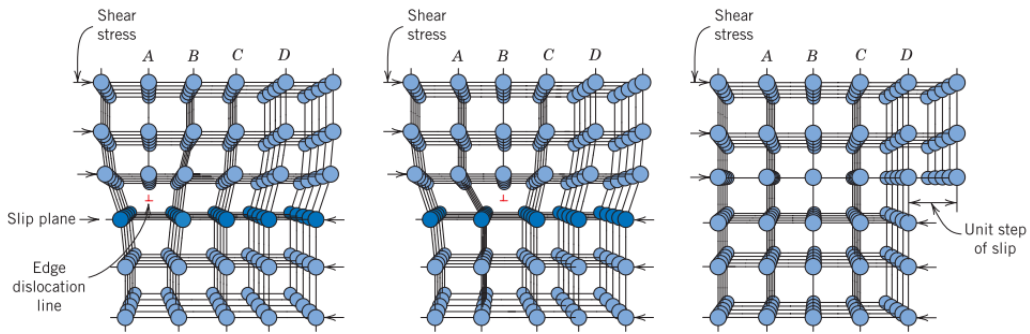


Figure 2.5: Glide of slip planes by dislocations. The figure from Ref. [3].

2.4 Slip Systems and Dislocation Movements

Plastic slip occurs in $[111]$ family planes and $\langle 110 \rangle$ family directions in FCC metals. Four $[111]$ planes and three $\langle 110 \rangle$ directions in each plane of FCC unit cell form 12 slip system,

Table 2.1.

Table 2.1: Slip systems in FCC metals.

Slip system No.	Slip plane	Slip direction
1	$[111]$	$\langle 01\bar{1} \rangle$
2	$[111]$	$\langle \bar{1}01 \rangle$
3	$[111]$	$\langle 1\bar{1}0 \rangle$
4	$[1\bar{1}\bar{1}]$	$\langle 0\bar{1}1 \rangle$
5	$[1\bar{1}\bar{1}]$	$\langle \bar{1}0\bar{1} \rangle$
6	$[1\bar{1}\bar{1}]$	$\langle 110 \rangle$
7	$[\bar{1}\bar{1}1]$	$\langle 0\bar{1}\bar{1} \rangle$
8	$[\bar{1}\bar{1}1]$	$\langle 101 \rangle$
9	$[\bar{1}\bar{1}1]$	$\langle \bar{1}10 \rangle$
10	$[\bar{1}1\bar{1}]$	$\langle 011 \rangle$
11	$[\bar{1}1\bar{1}]$	$\langle 10\bar{1} \rangle$
12	$[\bar{1}1\bar{1}]$	$\langle \bar{1}\bar{1}0 \rangle$

Glide of dislocations with Burgers vector (slip directions, $\langle 110 \rangle$ in FCC crystal, Figure 2.6a) needs high strain energy. As a consequence, dislocations decompose into two segments (partial dislocations, Figure 2.6b, 2.6c) to reduce strain energy and change the crystal structures. Disordered area is stacking fault with surface energy (stacking fault energy), Figure 2.6d. Balance between strain and stacking fault energy defines total dislocations decomposition possibility. Dislocation decomposition rarely happens in high stacking fault energy (SFE) materials such as aluminum and since total dislocations are more mobile (cross slip), these materials are more ductile. Main sources of materials softening and hardening under plastic deformation are dislocation annihilation and multi-

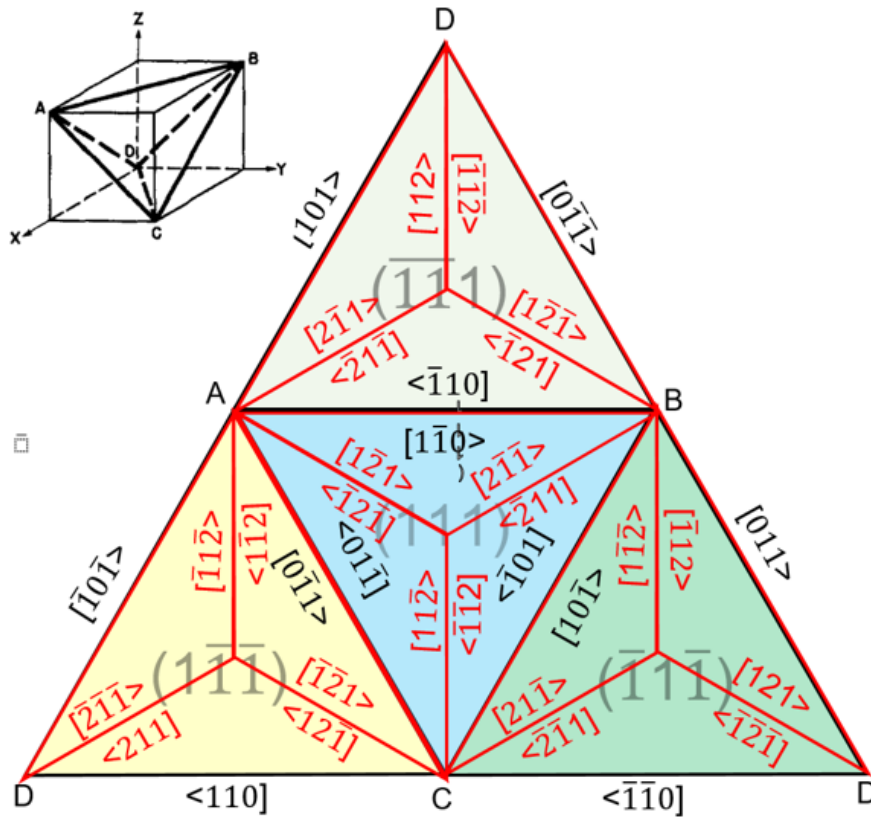


Figure 2.7: Total and partial dislocations of 12 slip systems in FCC metals.

2.5.1 Cross Slip and Annihilation

Dislocations trapped at obstacles can escape by changing the slip plane through climb (edge dislocations) and cross slip (screw dislocations). Since climb is less likely to occur in FCC metals at low homologous temperatures, edge segments remain sessile and screw segments evade via cross slip and annihilate each other, Figure 2.8.

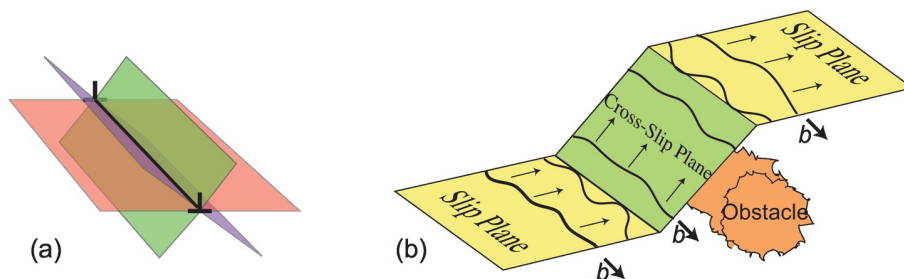


Figure 2.8: Cross slip of screw dislocations. The figure from Ref. [5].

Two dislocations in two connected slip planes (the Burgers vectors dot product=-2)

can cross slip and annihilate each other as,

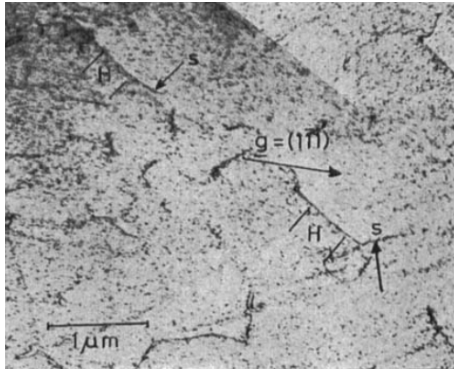
$$[111]\frac{1}{2}\langle 01\bar{1} \rangle + [\bar{1}\bar{1}1]\frac{1}{2}\langle 0\bar{1}1 \rangle = 0(\text{annihilation}) \quad (2.2)$$

2.5.2 Hirth locks

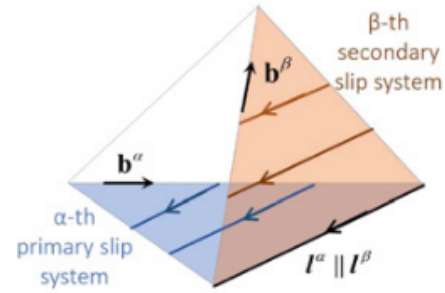
Two dislocations with zero dot product of their Burgers vectors (slip directions) are perpendicular to each other. The interaction of two perpendicular dislocations is a new one as,

$$[111]\frac{1}{2}\langle 01\bar{1} \rangle + [\bar{1}\bar{1}1]\frac{1}{2}\langle 0\bar{1}1 \rangle = \frac{1}{2}\langle 00\bar{1} \rangle, \quad (2.3)$$

Since the new dislocation, $\frac{1}{2}\langle 00\bar{1} \rangle$, is not in slip direction, it is immobile (sessile) dislocation and forms a strong lock which is known as a Hirth lock, Figure 2.9. Hirth locks are strong barriers to the movement of other dislocations and one of dominant sources of materials dislocation hardening [67].



(a)



(b)

Figure 2.9: Hirth locks (H). Figures from Ref. [6, 7].

2.5.3 Lommer-Cottrell locks

Interaction resultant of two partial dislocations in two different planes can be a new total one which is out of reactant dislocations planes as,

$$[111]\frac{1}{6}\langle\bar{1}2\bar{1}\rangle + [\bar{1}\bar{1}1]\frac{1}{6}\langle2\bar{1}1\rangle = \frac{1}{6}\langle110\rangle, \quad (2.4)$$

Since the new $\frac{1}{2}\langle110\rangle$ dislocation is not in $[111]$ nor in $[\bar{1}\bar{1}1]$ plane, it is immobile and called a Lommer-Cottrell lock, [68]. Lommer-Cottrell locks, Figure 2.10, are more common in low SFE materials in which partials are more favorable (lower energy), [4,5].

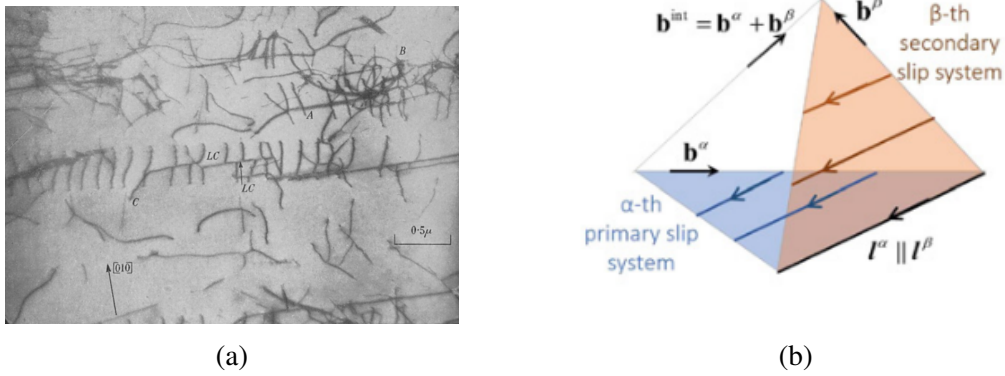


Figure 2.10: Lommer-Cottrell (LC). The figures from Ref. [6, 8].

All possible 144 dislocations interactions (12×12) in FCC metals are summarised in Figure 2.11. Dislocation interactions play a controlling role in materials' macroscopic behaviour and mesoscale dislocation substructure formation.

Slip Plane			Slip Dir. (Full Dislocations)			Partial Dislocation			Full Dislocation Interaction												
										1	2	3	4	5	6	7	8	9	10	11	12
1	1	1	0	1	-1	1 -1	1 2	-2 -1	1	-	Co	Co	CS	NG	NG	H	LC	NG	H	NG	LC
1	1	1	-1	0	1	-2 -1	1 -1	1 2	2	Co	-	Co	NG	H	LC	LC	H	NG	NG	CS	NG
1	1	1	1	-1	0	1 2	-2 -1	1 -1	3	Co	Co	-	NG	LC	H	NG	NG	CS	LC	NG	H
1	-1	-1	0	-1	1	1 -1	-1 -2	1 2	4	CS	NG	NG	-	Co	Co	H	NG	LC	H	LC	NG
1	-1	-1	-1	0	-1	-2 -1	-1 1	-1 -2	5	NG	H	LC	Co	-	Co	NG	CS	NG	LC	H	NG
1	-1	-1	1	1	0	1 2	2 1	-1 1	6	NG	LC	H	Co	Co	-	LC	NG	H	NG	NG	CS
-1	-1	1	0	-1	-1	-1 1	-1 -2	-2 -1	7	H	LC	NG	H	NG	LC	-	Co	Co	CS	NG	NG
-1	-1	1	1	0	1	2 1	-1 1	1 2	8	LC	H	NG	NG	CS	NG	Co	-	Co	NG	H	LC
-1	-1	1	-1	1	0	-1 2	2 1	-1 -1	9	NG	NG	CS	LC	NG	H	Co	Co	-	NG	LC	H
-1	1	-1	0	1	1	-1 1	1 2	2 1	10	H	NG	LC	H	LC	NG	CS	NG	NG	-	Co	Co
-1	1	-1	1	0	-1	2 1	1 -1	-1 -2	11	NG	CS	NG	LC	H	NG	NG	H	LC	Co	-	Co
-1	1	-1	-1	-1	0	-1 -2	-2 -1	-1 1	12	LC	NG	H	NG	NG	CS	NG	LC	H	Co	Co	-
										Coplanar		Hirth Lock		Lommer-Cottrell		Cross Slip		Not Likely or Glissile			

Figure 2.11: All possible 144 dislocation interactions (12×12) in FCC metals.

2.6 Dislocations Interactions and Mesoscale Substructure Formation

Various dislocation interactions are activated by loading single crystals in different orientations, Figure 2.12a. Effect of crystal orientation on the dislocations substructures of FCC metals has been extensively analyzed in TEM images for cyclic [9] and monotonic [1, 11, 61] loading, as shown by Figure 2.12b and 2.12c. The overall effect the interactions on mesoscale structures, which has been well established by TEM studies (Figure 2.12d), is as follows,

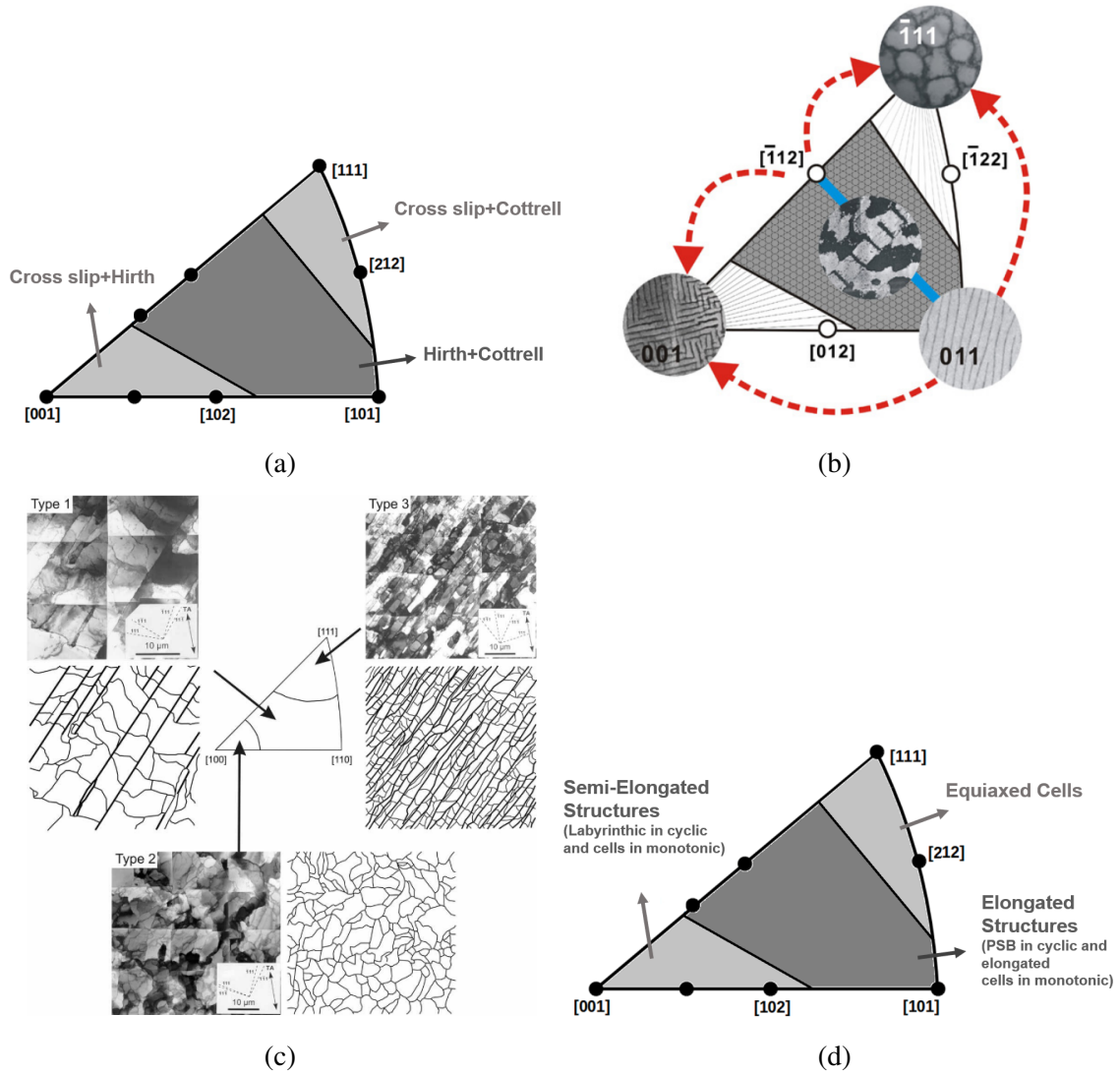


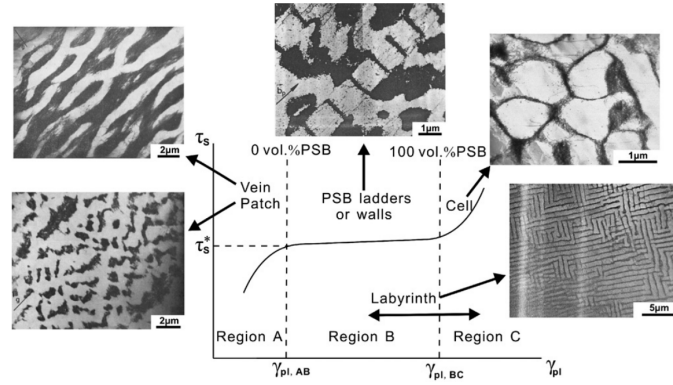
Figure 2.12: Effect of crystal orientation and dislocation interactions on the mesoscale dislocations substructure development. a) Activation of various dislocations interactions in different crystal orientations. b,c) Mesoscale dislocations substructures of crystals under b) cyclic and c) monotonic loadings. d) Overall effect. Figure b and c from from Ref. [1,9].

Hirth [67] computed relative interaction strengths for Hirth locks, Lommer-Cottrell locks and cross slip as 0.66, 0.33 and < 0.167 , respectively. We argue that the strength of Hirth locks impairs cross slip and results in elongated anisotropic structures from coplanar dislocation annihilation. Weaker Lommer-Cottrell locks are less effective in preventing cross slip induced annihilation and result in more equiaxed structures compared to those dominated by Hirth locks. Absence of both these locks along with profuse cross slip results in fully equiaxed isotropic cells. In the condition of same quantity of cross slip

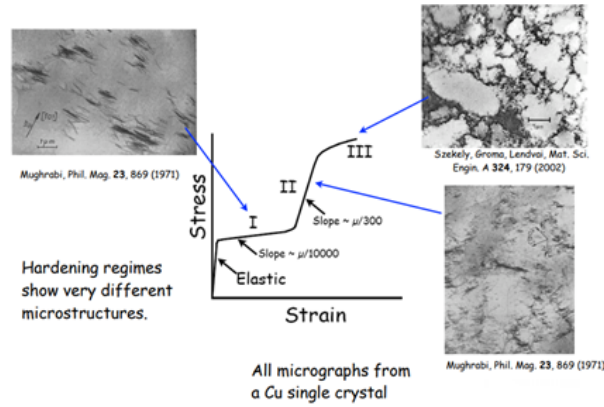
(screw) and Hirth locks (edge), due to more mobility of screw segments, the cross slip is dominant. Dominant cross slip in monotonic loading conditions forms equiaxed cells in crystals with abundant cross slip+Hirth locks. However, accumulation of Hirth locks during many cycles in cyclic deformations makes more elongated structures (labyrinthic) in these crystals (cross slip+Hirth). Mesoscale dislocation substructures formed by cross slip, Hirth and Lommer-Cottrell locks have been shown to define materials hardening behaviour, [9, 10].

2.7 Dislocations Substructures and Materials Hardening Behaviour

Relation between dislocations substructures and materials hardening behaviour has been demonstrated for cyclic [9] and monotonic [10] loading (Figure 2.13). Materials hardening is mainly controlled by mesoscale attributes such as dislocation cell wall fraction (f_w) [69], structures size or walls spacing (d_{struct}) [70] and structures aspect ratio, ($\eta = \frac{l_{struct}}{d_{struct}}$) [9, 42] which are shown in Figure 2.14.



(a)



(b)

Figure 2.13: Relation between dislocations substructures and materials hardening behaviour a) in cyclic and b) monotonic loading condition. Figure from Ref. [9].

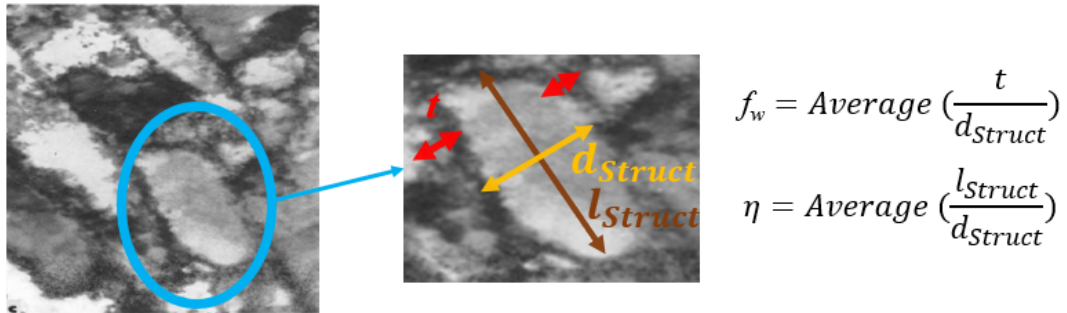
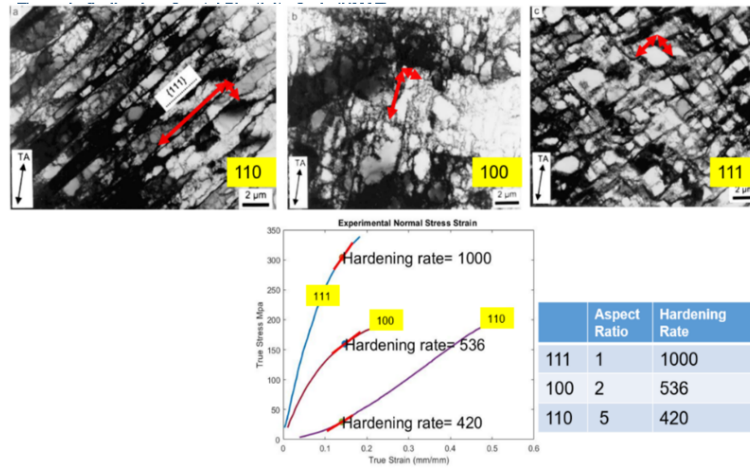


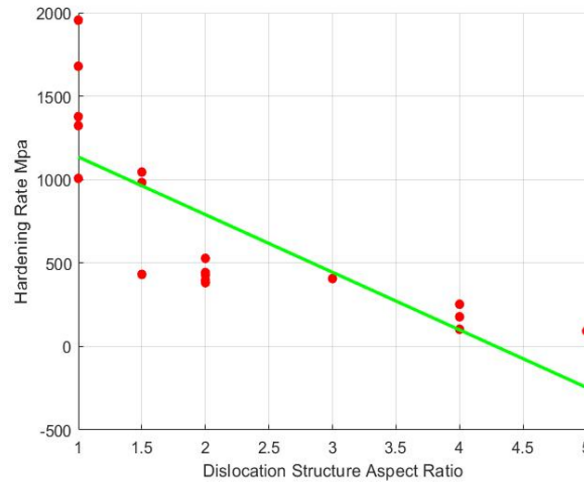
Figure 2.14: Explain of substructures attributes that define materials hardening: dislocation cell wall fraction (f_w), structures size or walls spacing (d_{struct}) and structures aspect ratio, ($\eta = \frac{l_{struct}}{d_{struct}}$). Average means repeating the measurements for all cells. TEM image from Ref. [10].

We measured dislocation aspect ratio, η , in TEM images of FCC metals and computed hardening rates of these structures (Figure 2.15, Details of measurements are explained in

Chapter 4). Analysis showed less hardening rates for elongated structures.



(a)



(b)

Figure 2.15: Relation between dislocations substructures aspect ratio, η , and hardening rate of FCC metals. Less hardening rates for elongated structures are apparent. Green line is linear fitting. TEM images from Ref. [11].

2.8 Stability of Dislocation Substructures in Cyclic Loading

As applied plastic shear strain amplitude increases to $\gamma_{pl,AB}$ in Figure 2.13a, Veins transform into PSBs which are stable up to $\gamma_{pl,BC}$ and then altered to cells and Labyrinthic structures at $> \gamma_{pl,BC}$. Labyrinthic is finally changed to cells at large enough strains. In-

fluence of applied plastic shear strain amplitude on dislocation substructures in single and multi-slip crystals is represented schematically in Figure 2.16. Accordingly, while intermediate metastable structures, i.e Veins, PSBs and Labyrinthic can be altered under monotonic overloads, cells are stable.

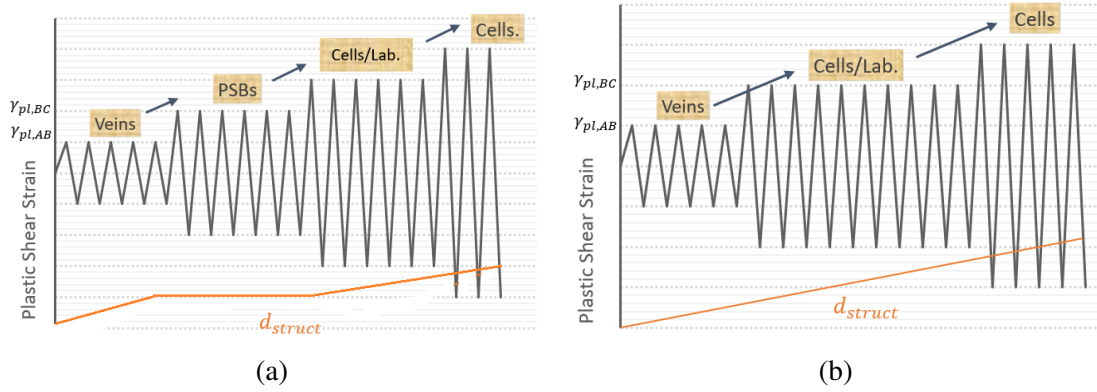


Figure 2.16: Influence of applied plastic shear strain amplitude on the dislocation substructures in a) Single and b) Multi-slip crystals under cyclic loading. As plastic shear strain amplitude increases, Veins transform into PSBs and the PSBs into cells and Labyrinthic structures. Labyrinthic is finally changed to cells at large enough strains.

Chapter 3

Crystal Plasticity Finite Element Modelling

Crystal plasticity constitutive models have been extensively used to represent the effects of crystallographic orientation on the mechanical response of metallic materials [71–74]. Myriads of phenomenological and physics-based formulations have quantified model parameters by fitting simulations to the macroscopic stress-strain response of polycrystals. This approach is sound to predict the homogenized response of polycrystals such as the roles of texture or the stochastic nature of cracking controlled by the microstructure. However, recent research efforts [75, 76] have demonstrated that parameters cannot be uniquely identified and cannot capture in detail the local response at or below the grain scale.

Despite being formulated to describe the crystalline response, crystal plasticity simulations have rarely been validated with single crystal experiments. One exception is the work by Arsenlis and Parks [77], who proposed a model that reproduced the response of Al single crystals up to 10% strain, but without comparing to polycrystals. More recently, Khan and coworkers [78] modelled the mechanical response of Al single crystals at different strain rates. Their work successfully predicted the crystal response up to 20% strain under quasistatic loading for two orientations with high Schmid factor and limited cross slip. However, the predictive power diminishes for higher strain rates, which highlights the difficulties in identifying parameters or model forms that work for various loading conditions. Moreover, their work also omits the comparison to polycrystal data.

Shawish et. al. [75] introduced an optimization scheme to identify crystal plasticity parameters through the simultaneous fitting of single- and poly-crystal experimental stress-strain of austenitic stainless steel. Their approach demonstrated that multiple sets of parameters can reproduce the experiments with similar accuracy as a result of shallow objective functions with multiple local minima. Furthermore, they showed that these parameters can yield different grain-level responses, which highlights the need for physics-based rather than mathematics-based strategies for parameter identification.

A different physics-based approach was proposed by Chandra et al. [79], who employed dislocation dynamic simulations to parameterize the thermal stress and the initial

hardening in crystal plasticity. Their work successfully reproduced the mechanical response of various crystals using a set of parameters for each orientation, which were subsequently averaged to predict the polycrystalline response. Although this approach does not predict single- and poly-crystals responses with a single parameterization, it demonstrates that by predicting single crystals we can approximate the behavior of polycrystals; notably, the inverse is not true in general. In the context of cyclic plasticity, Castelluccio and McDowell [66] also demonstrated that a crystal plasticity model capable of predicting single crystal responses has good predictive power over polycrystals. Their approach relied on the independent estimation of parameters characterized by the morphology of mesoscale dislocation substructures. Details of crystal plasticity modelling will be described in this chapter.

3.1 Constitutive Models

Following the foundations of crystal plasticity for large deformations [62, 65], total deformation gradient, $\mathbf{F}$, is characterized by the common elastic, $\mathbf{F}^e$, and plastic, $\mathbf{F}^p$, multiplicative decomposition, i.e.,

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p, \quad (3.1)$$

time derivative of plastic deformation gradient, $\dot{\mathbf{F}}^p$, relates to the isoclinic intermediate configuration plastic velocity gradient, $\mathbf{L}^p$, such that

$$\dot{\mathbf{F}}^p = \mathbf{L}^p \mathbf{F}^p = \sum_{\alpha=1}^{N_{\text{sys}}} \dot{\gamma}^{\alpha} (\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}), \quad (3.2)$$

where $\otimes$ is dyadic product, $\dot{\gamma}$ is shear rate while $\mathbf{s}^{\alpha}$ and $\mathbf{m}^{\alpha}$ correspond to the slip direction and slip plane normal of slip system α , respectively. Elastic deformation gradient is calculated,

$$\mathbf{F}^e = \mathbf{F} \cdot (\mathbf{F}^p)^{-1}, \quad (3.3)$$

to compute elastic Green strain tensor,

$$\mathbf{E}^e = \frac{1}{2} [(\mathbf{F}^e)^T \cdot \mathbf{F}^e - \mathbf{I}], \quad (3.4)$$

this tensor is then multiplied by fourth rank elasticity tensor with cubic symmetry, $\mathbf{C}$, to compute the 2nd Piola-Kirchhoff stress,

$$\sigma^{\text{PK2}} = \mathbf{C} : \mathbf{E}^e, \quad (3.5)$$

while the Cauchy stress is computed as,

$$\sigma = \frac{1}{\det(\mathbf{F}^e)} [\mathbf{F}^e \cdot \sigma^{\text{PK2}} \cdot (\mathbf{F}^e)^{-1}]. \quad (3.6)$$

Shearing rate on slip system α in Equation (3.2) is defined as a function of external stress and materials state through constitutive equations. Constitutive equations vary in defining the materials state. Two types of material constitutive models are common to implement in crystal plasticity models: phenomenological and physics-based constitutive models. We present these two types in the following.

3.1.1 Phenomenological Constitutive Models

In the phenomenological constitutive models, material state is mainly described by resolved shear stress on each slip system, τ^α . The shearing rate, $\dot{\gamma}^\alpha$, is computed as a function of resolved shear stress, τ^α , and slip resistance, τ_r^α ,

$$\dot{\gamma}^\alpha = f(\tau^\alpha, \tau_r^\alpha), \quad (3.7)$$

where the slip resistance, τ_r^α , is related to total shear, γ , and shear rate, $\dot{\gamma}$,

$$\tau_r^\alpha = g(\gamma, \dot{\gamma}). \quad (3.8)$$

Several authors proposed various equations for these functions (f and g), [62, 64, 65]. The most common functions are,

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{\tau_r^\alpha} \right|^{\frac{1}{m}} \text{sgn}(\tau^\alpha), \quad (3.9)$$

$$\dot{\tau}_r^\alpha = \sum_{\beta=1}^{N_{\text{sys}}} h_{\alpha\beta} \left| \dot{\gamma}^\beta \right|, \quad (3.10)$$

where $\dot{\gamma}_0$ and m are the reference shear rate and the rate sensitivity of slip, respectively. $h_{\alpha\beta}$ is the hardening matrix that reflects the effects of all slip systems (β) on the hardening of α slip system and formulated as,

$$h_{\alpha\beta} = q_{\alpha\beta} \left[h_0 \left(1 - \frac{\tau_r^\beta}{\tau_s} \right)^k \right], \quad (3.11)$$

in which h_0 , k and τ_s are the slip (self) and $q_{\alpha\beta}$ is the latent hardening parameters.

Phenomenological constitutive models are frequently used in crystal plasticity finite element models. However, they suffer from the drawback that physics of material is not explicitly included. We showed in the multiscale analysis in Chapter 2 that physical material states (substructures) define macroscopic behaviour. Hence, physics-based constitutive models need to reflect the relation between multiple scales mechanistic phenomenon.

3.1.2 Dislocation Density-based Constitutive Models

Physics-based constitutive models use internal physical variables to define material state. The most common internal physical variable reported to carry on the plastic deformation is dislocation density, [73, 80, 81]. The mobile dislocation densities, ρ_m^α , define the shearing rates, $\dot{\gamma}^\alpha$, in the physics-based models by Orowan equation (instead of Equation

(3.9)),

$$\dot{\gamma}^\alpha = \rho_m^\alpha b v^\alpha, \quad (3.12)$$

where, b and v are magnitudes of Burgers vector and average velocity of the mobile dislocations.

Effective shear stress, τ_{eff} , can be defined by resolved shear stress, τ^α , and slip resistance, τ_r^α ,

$$\tau_{eff} = \tau^\alpha - \tau_r^\alpha, \quad (3.13)$$

where the slip resistance, τ_r^α , is formulated by dislocation density,

$$\tau_r^\alpha = \alpha G b \sqrt{A \rho_m^\alpha}, \quad (3.14)$$

in which α and A are constants and G is materials shear modulus.

Dislocation density can not be easily measured in experiments. Hence, validation is often limited to macroscopic responses while they carry a large uncertainty on mesoscale variables and parameters. The large uncertainty of dislocation density demands for substructure-based crystal plasticity model with easy-to-measure and limited uncertainty internal state variables, i.e. substructures shape and size.

3.1.3 Substructure-based Constitutive Models

Orowan [82] computed the dislocation velocity in Equation (3.12) as,

$$v = l \nu \exp\left(\frac{-\Delta G}{k_B T}\right), \quad (3.15)$$

where l , ν , k_B and T are average distance between dislocations barriers, attempt frequency, Boltzmann constant and temperature, respectively. ΔG is Gibbs free activation energy of a dislocation which has been quantified by several approaches. The most fre-

quently used formulation of ΔG is, [83, 84] ,

$$\Delta G = F_0 \left(1 - \left[\frac{\tau}{s_0} \right]^p \right)^q, \quad (3.16)$$

in which F_0 is glide activation energy at 0 K and the s_0 is thermal stress and p and q are profile parameters. Some authors [85, 86] proposed similar formulations for ΔG . Combining Equations (3.12), (3.15) and (3.16) with a few modifications [63] gives the Arrhenius-type flow rule as,

$$\dot{\gamma}^\alpha = \rho_m^\alpha b l_{struct} v \exp \left(-\frac{F_0}{k_B T} \left\langle 1 - \left[\frac{\langle |\tau_{eff}^\alpha| \rangle}{s_t^0 \frac{\mu}{\mu_0}} \right]^p \right\rangle^q \right) \text{sgn}(\tau^\alpha - B^\alpha), \quad (3.17)$$

where μ and μ_0 are the shear modulus at temperature T and $0K$ and the Macaulay brackets follows $\langle G \rangle = 0$ if $G \leq 0$ or $\langle G \rangle = G$ if $G > 0$. l_{struct} is the substructures characteristic length (dislocation mean free path) which varies for different substructures, [42], and needs to be calibrated for monotonic and cyclic loadings. First term of the equation is the reference shear rate ($\dot{\gamma}_0 = \rho_m^\alpha b l_{struct} v$), Equation (3.12).

Equation (3.17) relates the local plastic shear rate induced by dislocation glide with local effective stress, τ_{eff}^α , driving the dislocation. Both magnitudes are associated with atomic scale unit processes, but relates to the mesoscale (finite element) level shear stress, τ^α , following,

$$\tau_{eff}^\alpha = \langle |\tau^\alpha - B^\alpha| - S^\alpha \rangle, \quad (3.18)$$

in which S^α corresponds to the local athermal stress and B^α to the intragranular back stress. We analysed dislocations substructures to find the physical sources of the Back and athermal stresses.

3.1.3.1 Substructure-based Back Stress

Bulk of a deformed material is divided into substructures wall and inner core. The plastic shear rate in a substructure with wall volume fraction of f_w is computed based on the shear rate in the wall, $\dot{\gamma}_p^w$, and in the inner core, $\dot{\gamma}_p^c$ as (rule of mixture),

$$\dot{\gamma}_p = f_w \dot{\gamma}_p^w + (1 - f_w) \dot{\gamma}_p^c, \quad (3.19)$$

Dislocation density within the walls is considerably higher than the inner core which makes the deformation of walls elastic, i.e. $\dot{\gamma}_p^w \approx 0$. The reversible elastic deformation in walls and the irreversible plastic deformation within the core produce residual (back) stress. Castelluccio and McDowell [66] derived that the back stress rate based on this assumption follows,

$$\dot{B}^\alpha = \frac{f_w}{1 - f_w} \frac{2\mu(1 - 2S_{1212})}{1 + 4S_{1212}f_{Hill}^S} \dot{\gamma}^\alpha, \quad (3.20)$$

in which f_{Hill}^S and S_{1212} are the Hill factor under shear deformation and the coefficient of substructures configuration, respectively. The common wall and core composition in monotonic and cyclic loadings substructures, makes Equation (3.20) applicable for both loadings conditions. However, due to the different substructures (Figure 2.13), the wall fraction, f_w , needs to be calibrated for monotonic and cyclic loadings.

3.1.3.2 Substructure-based Athermal Stress

Athermal stress is computed as the sum of the stress required to bow-out dislocations and the colinear dislocation-dislocation interaction strength [66],

$$S^\alpha = \alpha_{LE} \frac{\mu b}{2d_{struct}} + \mu b \sqrt{A_{\alpha\beta} \rho^\alpha}, \quad (3.21)$$

in which α_{LE} is the dislocation line energy coefficient and $A_{\alpha\beta}$ is dislocation interaction parameter, which is zero if $\alpha \neq \beta$ and a constant when $\alpha = \beta$ (colinear dislocation

interaction). Due to coexisting of the application area of this equation (inner core) in monotonic and cyclic, it is applicable for both loading conditions. This equation (4.12), defines the hardening of inner core while the hardening of walls is being counted by the back stress equation (3.20). The interactions among other dislocations, make strong locks (as described in chapter 2) and the locks change the structure. Hardening of structure change is being applied in the back stress equation and the first term of Equation (4.12). Accordingly, hardening of other dislocations (latent hardening) is not described in the second term of Equation (4.12), i.e, mobile dislocation density. Mobile dislocations density (ρ^α) evolves with the balance between dislocation multiplication, annihilation and cross slip such that [66],

$$\dot{\rho}^\alpha = \frac{K_{multi}}{bl_{struct}} |\dot{\gamma}^\alpha| - \frac{2y_s^{edge}}{b} \rho^\alpha |\dot{\gamma}^\alpha| + v_G \frac{d_{struct}}{d_0} \left(\phi_{cs} \sum_{\beta=1(\beta \neq \alpha)}^N \rho^\beta e^{(-V_{cs}^\alpha \frac{\mu b}{4\pi y_s^{screw}} - |\tau^\alpha - B^\alpha| \frac{1}{K_B T})} - (1 - \phi_{cs}) \sum_{\beta=1(\beta \neq \alpha)}^N \rho^\beta e^{(-V_{cs}^\beta \frac{\mu b}{4\pi y_s^{screw}} - |\tau^\beta - B^\beta| \frac{1}{K_B T})} \right). \quad (3.22)$$

Here, K_{multi} scales the number of dislocations produced after applying a certain plastic shear strain while y_s^{edge} and y_s^{screw} are the annihilation distances for edge and screw dislocations, respectively. Cross-slip efficiency parameter ϕ quantifies the likelihood for dislocation annihilation while cross slipping and V_{cs} represents cross slip activation volume. Because the dislocation evolution mechanisms are same for monotonic and cyclic, Equation (3.22) works for both loading conditions.

Mean spacing of sessile dislocations walls, d_{struct} , is being calculated by the maximum amount of resolved shear stress among all slip systems, τ_{max} , in the so-called similitude relation [70, 87],

$$d_{struct} = K_{struct} \frac{\mu b}{\tau_{max}}, \quad (3.23)$$

in which K_{struct} is a similitude coefficient. Castelluccio and McDowell [66] further pro-

posed to relate dislocations mean free path to d_{struct} ,

$$l_{struct} = \eta d_{struct}, \quad (3.24)$$

where the substructure aspect ratio, η , is a mesoscale attribute that describes dislocation structure morphology and depends on the crystallographic orientation and deformation [88].

Since characteristic substructures are different for monotonic and cyclic (Figure 2.13), the structural parameters (d_{struct} , η and f_w) need to be parametrised for each loading condition. Castelluccio and McDowell [66] proposed a mesoscale model for cyclic loading condition to compute the mentioned structural parameters as functions of dislocation interactions (slip systems). Chapter 4 develops a model to predict the parameters for monotonic loading.

3.2 Numerical Implementation

The constitutive equation (Equation (3.17)) was solved in Abaqus 2020 making use of the user material subroutine (UMAT). Abaqus computes total deformation gradient, $\mathbf{F}$, by tracking the relative displacements of finite elements nodes (integration points),

$$\mathbf{F} = \frac{\partial \mathbf{x}_i}{\partial \mathbf{X}_j}. \quad (3.25)$$

Macroscopic Cauchy stress at current time increment, $t + \Delta t$ (t represents previous time step and $t + \Delta t$ corresponds to current new time step), computes as,

$$\boldsymbol{\sigma}_{t+\Delta t} = \frac{1}{\det(\mathbf{F}_{t+\Delta t}^e)} [\mathbf{F}_{t+\Delta t}^e \cdot \boldsymbol{\sigma}_{t+\Delta t}^{PK2} \cdot (\mathbf{F}_{t+\Delta t}^e)^{-1}], \quad (3.26)$$

in which 2nd Piola-Kirchhoff stress, $\boldsymbol{\sigma}_{t+\Delta t}^{PK2}$, is being calculated as,

$$\boldsymbol{\sigma}_{t+\Delta t}^{PK2} = \mathbf{C} : \mathbf{E}_{t+\Delta t}^e, \quad (3.27)$$

where $\mathbf{C}$ is fourth rank elasticity tensor with cubic symmetry and $\mathbf{E}_{t+\Delta t}^e$ is Green strain tensor,

$$\mathbf{E}_{t+\Delta t}^e = \frac{1}{2} [(\mathbf{F}_{t+\Delta t}^e)^T \cdot \mathbf{F}_{t+\Delta t}^e - I]. \quad (3.28)$$

By using the decomposition of total deformation gradient to elastic and plastic part ($\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$), the elastic deformation gradient at current time increment, $\mathbf{F}_{t+\Delta t}^e$, computes as,

$$\mathbf{F}_{t+\Delta t}^e = \mathbf{F}_{t+\Delta t} (\mathbf{F}_{t+\Delta t}^p)^{-1}, \quad (3.29)$$

where $\mathbf{F}_{t+\Delta t}$ is provided by Abaqus and $\mathbf{F}_{t+\Delta t}^p$ is being computed in the UMAT by velocity gradient, $\mathbf{L}_{t+\Delta t}$,

$$\mathbf{F}_{t+\Delta t}^p = \mathbf{L}_{t+\Delta t}^p \Delta t \mathbf{F}_t^p, \quad (3.30)$$

and the velocity gradient, $\mathbf{L}_{t+\Delta t}$, relates to local shear rates, $\dot{\gamma}^\alpha$,

$$\mathbf{L}_{t+\Delta t}^p = \sum_{\alpha=1}^{N_{\text{sys}}} \dot{\gamma}_{t+\Delta t}^\alpha (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha). \quad (3.31)$$

Local shear rates, $\dot{\gamma}_{t+\Delta t}^\alpha$, are the solution of a system of 12 equations (Equation (3.17)) for 12 slip systems of FCC metals. We used Newton-Raphson Method to solve equations with an implicit scheme.

3.2.1 Newton-Raphson Method

Maximum shear stress, τ_{max} , is used to compute dislocation substructures wall spacing, d (Equation (3.23)). Other substructure parameters, η and f_w , are computed based on plastic shear on slip systems from previous time step with the mesoscale models. Substitution of this shear stress with the previous steps athermal and back stress in Equation (3.17) gives a set of shear rates ($\dot{\gamma}$). Computed shear rates are the initial guess for the Newton-Raphson solution of the Equation (3.17).

Following the numerical integration scheme proposed by McGinty [89], the algorithm solves Equation (3.17) with an implicit solution for each integration point at each time

increment. The resolved shear stress, the back stress, and the athermal stress depend on the values of $\dot{\gamma}^\alpha$ and they are solved simultaneously by a Newton-Raphson method [89] that defines the slip system level function,

$$f^\alpha = \dot{\gamma}^\alpha - \dot{\gamma}_0^\alpha \exp \left(-\frac{F_0}{k_b T} \left\langle 1 - \left[\frac{\langle |\tau_{eff}^\alpha| \rangle}{s_t^0 \frac{\mu}{\mu_0}} \right]^p \right\rangle^q \right) \text{sgn}(\tau_{eff}^\alpha), \quad (3.32)$$

in which the values of $\dot{\gamma}^\alpha$ that minimize f^α correspond to the solution of this non-linear systems of equations. The Newton-Raphson computes the unknown $\dot{\gamma}^\alpha$ by iteratively solving the equations along with the explicit integration of the back stress and dislocation density evolution ((Equations (3.20), (4.12) and (3.22)) [89]). The new values of the shear rates, $\dot{\gamma}$, in the iterative solution is updated by,

$$-\sum_{\beta=1}^{N_{sys}} \frac{\partial f^\alpha}{\partial \dot{\gamma}^\beta} \Delta \dot{\gamma}^\beta = f^\alpha, \quad (3.33)$$

The solution algorithm is shown in Figure 3.1. The $\frac{\partial f^\alpha}{\partial \dot{\gamma}^\beta}$ term in Equation (3.33), is the Jacobian of the Newton-Raphson function. We used both numerical and analytical Jacobians to compare the results and assure the correct working of the numerics.

3.2.2 Analytical Jacobian

Analytical Jacobian of the Newton-Raphson function is computed as,

$$J_{\alpha\beta} = \frac{\partial f^\alpha}{\partial \dot{\gamma}^\beta} = \frac{\partial \dot{\gamma}^\alpha}{\partial \dot{\gamma}^\beta} - \dot{\gamma}_0^\alpha \frac{\partial (G1^\alpha)}{\partial \dot{\gamma}^\beta} \exp(G1^\alpha), \quad (3.34)$$

$$G1^\alpha = -\frac{F_0}{k_b T} \left\langle 1 - G2^\alpha \right\rangle^q, \quad (3.35)$$

where the first term is 1 if $\alpha = \beta$ and 0 otherwise, and the second term,

$$\frac{\partial (G1^\alpha)}{\partial \dot{\gamma}^\beta} = \frac{q F_0}{k_b T} \frac{\partial (G2^\alpha)}{\partial \dot{\gamma}^\beta} \left\langle 1 - G2^\alpha \right\rangle^{q-1}, \quad (3.36)$$

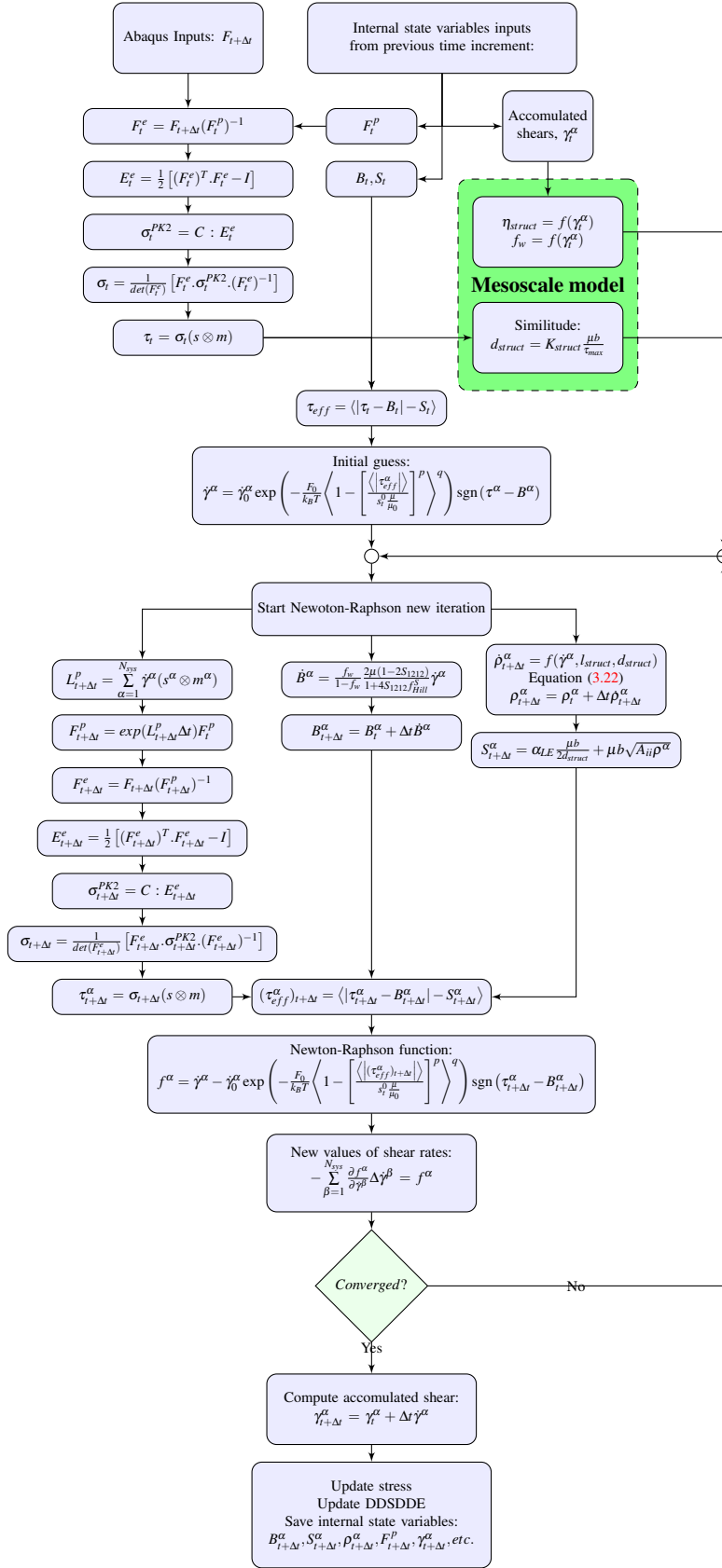


Figure 3.1: Flowchart for the numerical implementation

$$\frac{\partial (G2^\alpha)}{\partial \dot{\gamma}^\beta} = \frac{p}{s_t^0 \frac{\mu}{\mu_0}} \frac{\partial (\tau_{eff}^\alpha)}{\partial \dot{\gamma}^\beta} \left[\frac{\langle |\tau_{eff}^\alpha| \rangle}{s_t^0 \frac{\mu}{\mu_0}} \right]^{p-1}, \quad (3.37)$$

$$\frac{\partial (\tau_{eff}^\alpha)}{\partial \dot{\gamma}^\beta} = \frac{\partial (\langle |\tau^\alpha - B^\alpha| - S^\alpha \rangle)}{\partial \dot{\gamma}^\beta} = \left(\frac{\partial \tau^\alpha}{\partial \dot{\gamma}^\beta} - \frac{\partial B^\alpha}{\partial \dot{\gamma}^\beta} \right) \text{sgn}(\tau^\alpha - B^\alpha) - \frac{\partial S^\alpha}{\partial \dot{\gamma}^\beta}, \quad (3.38)$$

here if $|\tau^\alpha - B^\alpha| - S^\alpha < 0$ then $\frac{\partial \tau_{eff}^\alpha}{\partial \dot{\gamma}^\beta} = 0$ and $J_{\alpha\beta} = \frac{\partial \dot{\gamma}^\alpha}{\partial \dot{\gamma}^\beta}$. Following the chain rule,

$$\frac{\partial \tau^\alpha}{\partial \dot{\gamma}^\beta} = \left(\frac{\partial \tau^\alpha}{\partial \sigma} \right) \cdot \left(\frac{\partial \sigma}{\partial \sigma^{PK2}} \right) \cdot \left(\frac{\partial \sigma^{PK2}}{\partial E^e} \right) \cdot \left(\frac{\partial E^e}{\partial F^e} \right) \cdot \left(\frac{\partial F^e}{\partial F^p} \right) \cdot \left(\frac{\partial F^p}{\partial L_0^p} \right) \cdot \left(\frac{\partial L_0^p}{\partial \dot{\gamma}^\beta} \right), \quad (3.39)$$

in which the terms of the right side correspond to Equations (2.1), (3.6), (3.5), (3.4), (3.3) and (3.2), respectively. The result can be approximated to [89],

$$\frac{\partial \tau^\alpha}{\partial \dot{\gamma}^\beta} = -(s^\alpha \otimes m^\alpha) : C_0 : (s^\beta \otimes m^\beta), \quad (3.40)$$

and for the back stress using the Equation (3.20) leads to,

$$\frac{\partial B^\alpha}{\partial \dot{\gamma}^\beta} = \Delta t \frac{\partial \dot{B}^\alpha}{\partial \dot{\gamma}^\beta} = \Delta t \frac{f_w}{1 - f_w} \frac{2\mu(1 - 2S_{1212})}{1 + 4S_{1212}f_{Hill}^S}, \quad (3.41)$$

for the athermal stress Equations (4.12) and (3.22),

$$\frac{\partial S^\alpha}{\partial \dot{\gamma}^\beta} = \frac{\partial S^\alpha}{\partial \rho^\alpha} \cdot \frac{\partial \rho^\alpha}{\partial \dot{\gamma}^\beta} = \frac{\partial S^\alpha}{\partial \rho^\alpha} \cdot \Delta t \frac{\partial \dot{\rho}^\alpha}{\partial \dot{\gamma}^\beta} = (\mu b A_{ii} / \sqrt{A_{ii} \rho^\alpha}) \cdot \left(\frac{K_{multi}}{bl_{struct}} - \frac{2y_s^{edge}}{b} \rho^\alpha \right) \text{sgn}(\dot{\gamma}^\alpha). \quad (3.42)$$

3.2.3 Numerical Jacobian (Broydens Method)

Complex form of the analytical Jacobian demands a numerical one for testing and debugging. In the Broydens numerical Jacobian method, [90], very small values are added to the shear rates, $(\dot{\gamma}^\alpha + \delta \dot{\gamma}^\alpha)$, at the first Newton-Raphson increment ($n = 1$), to compute

internal variables ($\tau_{n=1}(\dot{\gamma}^\alpha + \delta \dot{\gamma}^\alpha)$, $B_{n=1}(\dot{\gamma}^\alpha + \delta \dot{\gamma}^\alpha)$ and $S_{n=1}(\dot{\gamma}^\alpha + \delta \dot{\gamma}^\alpha)$ and the function value, $f_{n=1}(\dot{\gamma}^\alpha + \delta \dot{\gamma}^\alpha)$. The Jacobian at the next Newton-Raphson increment ($n > 1$) is being computed as,

$$J_n^{\alpha\beta} = J_{n-1}^{\alpha\beta} + \frac{\Delta f_n^\alpha - J_{n-1}^{\alpha\beta} \Delta \dot{\gamma}_n^\alpha}{\|\Delta \dot{\gamma}_n^\alpha\|^2} (\Delta \dot{\gamma}_n^\alpha)^T. \quad (3.43)$$

3.2.4 Convergence Criteria

Three convergence criteria are common in the solution of non-linear systems of equations, [89]. The first criterion uses the change of a set of the solutions ($\dot{\gamma}^\alpha$, $\alpha = 1, 2, \dots, 12$) to stop the Newton-Raphson loop and accept the values,

$$Error = \text{Max} \left| \frac{\Delta \dot{\gamma}^\alpha}{\dot{\gamma}^\alpha} \right| < tolerance, \quad (3.44)$$

the set of solutions by this criterion may not minimize the Newton-Raphson function values. Hence the second criterion based on the least square minimization of the function values is,

$$Error = \sqrt{\frac{1}{N_{sys}} \sum_{\alpha=1}^{N_{sys}} (f^\alpha)^2} < tolerance, \quad (3.45)$$

this criterion is satisfied in the probable existence of local minima, while the error of some of the components of the set of solutions may not be negligible. To avoid trapping into the local minima, the third criterion based on both the solutions and the function values proposed,

$$Error = \sqrt{\frac{1}{N_{sys}} \sum_{\alpha=1}^{N_{sys}} \left(\frac{\dot{\gamma}^\alpha}{\dot{\gamma}_{max}} f^\alpha \right)^2} < tolerance, \quad (3.46)$$

we used this criterion in our UMAT.

3.2.5 Line Search and Time Step Subincrementation

The solution divergence is a common challenge in solving non-linear system of equations by Newton-Raphson method. The large Newton-Raphson increments (local) and the large time step increments (global) are the sources of the solution divergence.

The new updated values, $\dot{\gamma}$, halved after each Newton-Raphson increment in the line search technique to mitigate the local divergence. The breakdown process continues until the convergence criterion is satisfied (small enough Newton-Raphson increments). The material internal variables and the function values, are also redefined after each line search application, [89].

To mitigate global divergence, the first strategy is to break down the variable that depends on Abaqus time step increments, i.e. total deformation gradient, Equation (3.1). The total deformation gradient continues to be halved till convergence criterion is satisfied in time step subincrementation. However, the Abaqus needs to be forced to decrease time step by PNEWDT command (the second strategy) if divergence persists after numerous subincrementations, [89].

3.2.6 Materials Global Jacobian, DDSDDDE

The outputs of the UMAT subroutine are stress, σ , and the Jacobian of the hardening rate, $\frac{\partial \Delta \sigma}{\partial \Delta \epsilon}$ (DDSDDDE or tangent stiffness tensor). Abaqus uses the stress and the DDSDDDE to compute the strains and deformation gradient (the UMAT inputs), [91].

$$\frac{\partial \Delta \sigma}{\partial \Delta \epsilon} = \frac{\partial \frac{\Delta \sigma}{\Delta t}}{\partial \frac{\Delta \epsilon}{\Delta t}} = \frac{\partial \dot{\sigma}}{\partial \dot{\epsilon}}, \quad (3.47)$$

In this work, the elastic moduli tensor is used as the global Jacobian ($DDSDDDE = \frac{\partial \Delta \sigma}{\partial \Delta \epsilon} =$ C)

Chapter 4

Substructure-Sensitive Crystal

Plasticity Model for Monotonic Loading

This chapter innovates with a substructure-sensitive crystal plasticity approach that predicts the monotonic response of single and poly-crystals, simultaneously. We rely on a physics-based strategy for the independent identification of parameters by assimilating changes in the mesoscale substructure to a phase transformation among stable configurations. We demonstrate that mesoscale parameters are intrinsic to the structures and the same values apply to different FCC metals such as Cu, Ni and Al at similar homologous temperatures. Hence, mesoscale parameters are material-invariant for metals with similar dislocation substructures. As a result, our crystal plasticity approach is intrinsically built to predict single- and poly-crystalline response across systems with similar dislocation substructures without the need for unique single crystal experimental data for calibration.

4.0.1 Substructure-Sensitive Crystal Plasticity Model

In the absence of grain boundaries and precipitates, strain hardening in metallic materials arises from the production of dislocation locks with different strengths (e.g., Lomer–Cottrell, Hirth). Hähner [92] and Kuhlmann and Comins [93] argued that screw and edge dislocations trapped in dislocation locks can evade by cross slip and climb, respectively. Since climb is less likely to occur in FCC metals at low homologous temperatures, edge segments remain sessile and form immobile athermal dislocation walls. On the other hand, screw segments evade from locks via cross slip to annihilate and make dislocation free regions. This formation mechanism relies on cross slip and results in thermally-activated wall structures: Profuse cross slip enables equiaxed dislocation structures and refined walls upon increasing temperature or strain. On the contrary, at low strain, low temperature, or high Schmid factor, cross slip is not favored, resulting in athermal and anisotropic wall structures.

Thermal and athermal dislocation structures coexist throughout the stress-strain curve. Upon loading, initial coplanar dislocations lead to elongated athermal structures that eventually transition into more equiaxed cells due to the activation of profuse cross slip. As a result, the mechanical response presents multiple hardening stages associated with dif-

ferent structures. Hansen et al, [1, 61] identified three types of structures (I, II and III) according to their orientations and related their hardening to their dominant dislocation substructure. A similar relation between hardening and structures was found by Sard and Weil, [10], who showed that low and high hardening rates relates to elongated and equiaxed cell structures, respectively. As shown by Castelluccio et al. [66] for cyclic deformation, the partition of plastic deformation among slip system can serve as a predictor for the dominant substructure morphology. Next, we present a model that predicts the morphology of the dominant dislocation structure from the partition of plasticity across slip planes.

4.0.2 Mesoscale Structure Identification

Dislocation structures evolve upon loading according to their relative stability. Early on Holt [94] proposed that such a process can be assimilated to a spinodal decomposition. We follow a similar spirit and propose a substructure-sensitive approach for which the transition is analogous to a phase transformation in between three stable states that correspond to the structure types described by Hansen [1, 61]. Hence, we assume that each type of structure has intrinsic characteristic attributes $\eta^\#$ and $f_w^\#$, while the partition and accumulation of plasticity modulate the transition through these states.

We hypothesize that the strength of the dislocation interactions [67] determines the likelihood of a structure to being stable. Hirth [67] computed the relative interaction strengths for Hirth locks, Cottrell locks and cross slip as 0.66, 0.33 and < 0.167 , respectively. We argue that the strength of Hirth locks impairs cross slip and results in elongated anisotropic cells from coplanar dislocation annihilation. Weaker Cottrell locks are less effective in preventing cross slip induced annihilation and result in more equiaxed structures compared to those dominated by Hirth locks. The absence of both these locks along with profuse cross slip results in fully equiaxed isotropic cells.

Upon loading, dislocation production, lock formation, and cross slip annihilation results in a gradual transition among structures. We can equate this response to a transition

from coplanar dislocations (anisotropic and athermal) into cross slip dominated structures (equiaxed and thermal). We assume that the partition of plastic shear in the corresponding lock planes serves as a predictor for the transition among structures. The plastic shear partition refers to the accumulated shear strain on slip planes that form various locks or cross slip with respect to the most active slip plane. Hence, equiaxed cells (Type III) appear when the plastic shear strain on the cross slip plane associated to the most active slip plane exceeds the critical value γ_{Cr} . Similarly, Type I and II structures will appear depending on the relative accumulation of shear strain on planes that form Hirth or Cottrell locks, provided the cross slip threshold is not exceeded.

Figure 4.1 summarizes the strategy to identify the dominant structure with a flowchart that depends on the equivalent shear strain (γ^{eq}),

$$\gamma^{eq} = \gamma_0^{eq} \left(\gamma_{Max} + \gamma_{Cottrell} - \frac{1}{2} \gamma_{Hirth} \right) \quad (4.1)$$

which corresponds to the weighted summation of the accumulated shear on the most active slip system and its corresponding Hirth and Cottrell slip systems. Also γ_0^{eq} and γ_{Max} are a scaling coefficient and maximum amount of shear among all slip systems, respectively. The factor $\frac{1}{2}$ arises from the strength of Hirth locks being approximately twice of that for Cottrell locks. The dislocation wall volume fraction depends on the plastic strain accumulation across multiple slip plane as computed on Figure 4.1. The error function is characteristic of smooth phase transformations [95] and modulates the roles of Hirth or Cottrell locks on preventing cross slip for Types I and II structure. These equations result in a delay in the transformation into equiaxed cells from Hirth locks while shear strains on slip planes associated with Cottrell locks accelerate it.

4.1 Parameter Identification

To mitigate the lack of parameter uniqueness in crystal plasticity we seek a physics-based rather than a pure mathematical strategy [96]. In practice, parameter ambiguity arises

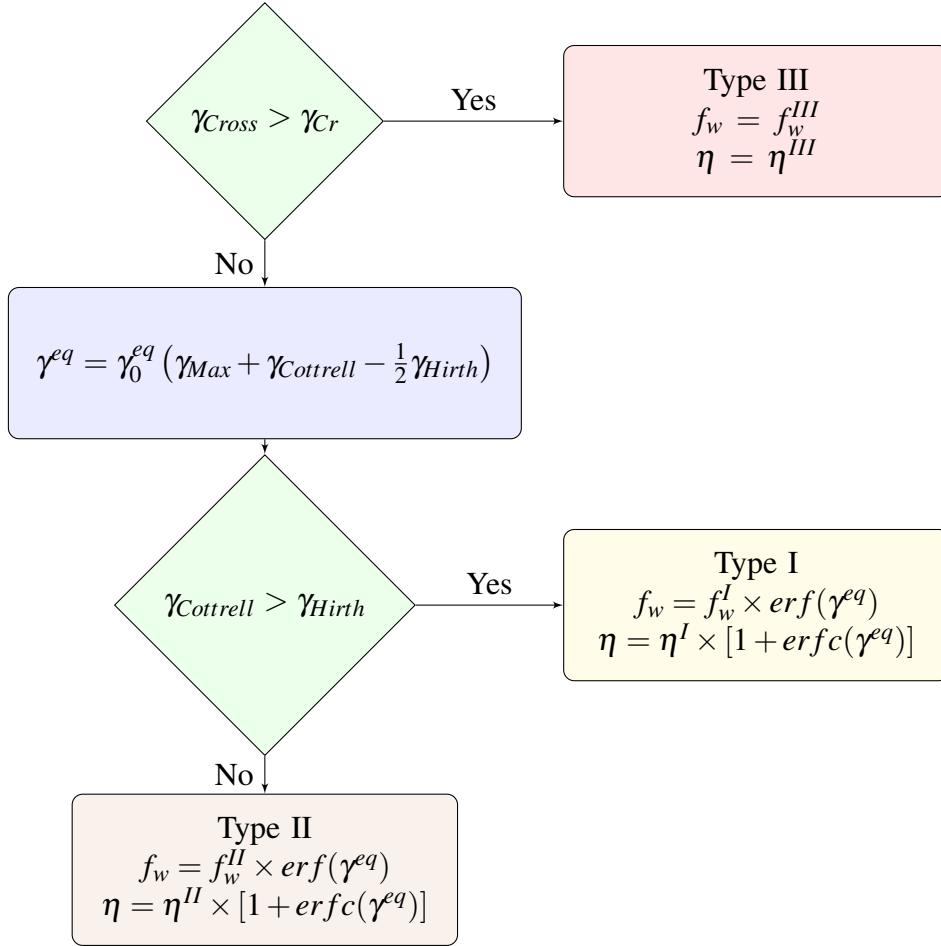


Figure 4.1: Flowchart for the identification of mesoscale attributes η and f_w . Type III structures (equiaxed cells) have constant wall fraction and aspect ratio, and they develop upon profuse cross slip from the dominant slip system. For Type I and II (elongated cells), η and f_w are modulated by error function. The accumulated shear strain on the most active slip system and on the slip planes that form Hirth and Cottrell locks control the evolution of the structures. TEM images adapted from [10, 12]

from limited experimental data available to identify a large number of parameters. Thus, we mitigate this problem by integrating experimental data for multiple metals with identical mechanisms.

We further differentiate between low and high sensitivity parameters based on their expected modelling impact upon changes within their independent value bounds. In this sense, parameters with relatively low uncertainty can be simply regarded as exact. However, atomic and mesoscale scale processes parameters that describe the response of a statistical ensemble are typically known with limited accuracy. For these high uncertainty parameters, we make an informed guess based on the value ranges reported on the literature.

4.1.1 Parameters with Low Expected Sensitivity

The Burgers vector, b , the shear modulus at room and 0K temperature, μ and μ_0 , and the elastic constants, C_{11} , C_{12} , and C_{44} are regarded as low uncertainty and low sensitivity. Similarly, assume that the initial dislocation density, ρ_0 , and initial wall spacing, d_0 , correspond to those from well annealed materials [97]. Table 4.1 summarizes the values from the low uncertainty parameters for Al, Cu and Ni.

Table 4.1: Material parameters with low uncertainty for Al, Cu and Ni. The shear modulus and elastic constants were computed based on Vigot [50], and Varshni [51] for Cu and Ni at 298K and Al at 77K.

Parameter	Values
Burgers Vector, b , (m)	2.56×10^{-10} [66]
Initial dislocation density, ρ_0 , ($\frac{1}{m^2}$)	10^8
Initial wall spacing, d_0 , (μ)m	12
Shear modulus at room temperature, μ , (GPa)	45 (Cu) 28 (Al) 80 (Ni) [50, 51]
Shear modulus at 0K, μ_0 , (GPa)	55(Cu) 31.6 (Al) 92 (Ni) [50, 51]
Elastic Constant, C_{11} , (GPa)	161(Cu) 115 (Al) 249(Ni) [50, 51]
Elastic Constant, C_{12} , (GPa)	119(Cu) 62 (Al) 155(Ni) [50, 51]
Elastic Constant, C_{44} , (GPa)	75(Cu) 31 (Al) 114.6(Ni) [50, 51]

4.1.2 Atomic Scale Process Parameters

The glide activation energy (F_0) and the thermal stress at 0 K (s_0^t) carry significant uncertainty associated with the thermal activation required for a dislocation to surpass an atomic-scale obstacle and enable glide. Ashraf and Castelluccio [26] considered the change in yield stress with temperature to develop an independent parameterization of F_0 and s_0^t for various materials, including Cu, Ni and Al. Similarly, atomistic and experimental analyses have estimated the annihilation distance for edge dislocations, y_{edge}^s , to be in the range between 0.5 to 5.0 nm at room temperature [98] while that for screw dislocations y_{screw}^s is in the range of tens to hundreds of nanometers [99]. Cross slip also depends on several parameters such as the jump frequency, $\nu_G = 10^{12} s^{-1}$ [66] and the activation reference volume, $V_{cs}^0 = 1000b^3$ [100]. Table 4.2 summarizes the values of atomic scale parameters used in the model.

Table 4.2: Material atomic scale parameters considered in the crystal plasticity model.

Parameter	Values
Glide activation energy, $F_0(\frac{KJ}{Mole})$	145(Cu) 150(Ni) 100(Al) [26]
Athermal stress at 0 K, s_0^t (MPa)	10 (Cu), 30(Ni), 10(Al) [26]
The profile parameters, p	0.67 [26]
The profile parameters, q	1.5 [26]
The annihilation distances for edge dislocations, y_{edge}^s (nm)	2.0(Cu) 2.0(Ni) 4(Al, 77K) [98]
The annihilation distances for edge dislocations, y_{screw}^s (nm)	40.0(Cu) 40.0(Ni) 80.0(Al, 77K) [99]
The cross slip frequency, ν (s^{-1})	10^{12} [66]
Cross slip activation volume, V_{cs}^0 (MPa)	1.67×10^{-26} [100]
Cross-slip efficiency parameter, ϕ	0.5 [66]

4.1.3 Mesoscale Parameters

We now consider parameters associated with the line and structure character of dislocations, which are summarized in Table 4.3. All parameters fall within the range from independent estimations using models and experiments. For example, the colinear dislocation interaction coefficient, A_{ii} , has been estimated by numerous experiments and dislocation dynamic simulations [42, 101] to be between 0.1 to 0.15. Sauzay and Kubin [70, 87] also analyzed the similitude coefficient, K_{struct} , and concluded it has a value between five and ten under monotonic loading for a wide range of FCC metals. Similarly, the line tension, α_{LE} is associated with the stress required to create new dislocations and has been estimated in the range of 0.5 to 1.5 [102, 103]. Furthermore, the dislocation multiplication factor, K_{multi} , has been estimated in the range between one to four by Tabata et al. [102] and between one and two by Castelluccio and McDowell [66].

Following an extensive characterization of structures from TEM images for various FCC metals (see 4.1.4), we estimated the intrinsic $\eta^\#$ and $f_w^\#$ for each type of structure. The results on Figure 4.2 demonstrate that Type II structures are the most anisotropic and correspond to elongated cells typically with $3 < \eta^{II} < 10$ as a result of strong Hirth locks. Type I structures are controlled by weaker Cottrell typically with $1 < \eta^I < 5$. In the absence of these locks along with profuse cross slip across result in fully equiaxed cells (Type III, $\eta^{III} \simeq 1.0$).

Similarly, we evaluated the wall fraction parameter for each structure type and concluded that in all cases f_w is in the range between 0.2 to 0.25 for homologous temperatures in between 0.1 to 0.2. Notably, the wall fraction of thermal structures (e.g., Type III f_w^{III}) is likely to depend on the temperature.

4.1.4 Experimental Mesoscale Attributes

By leveraging on extensive TEM images on the literature we estimated the mesoscale parameters for the three types of dislocation structures. Figure 4.3 shows experimental

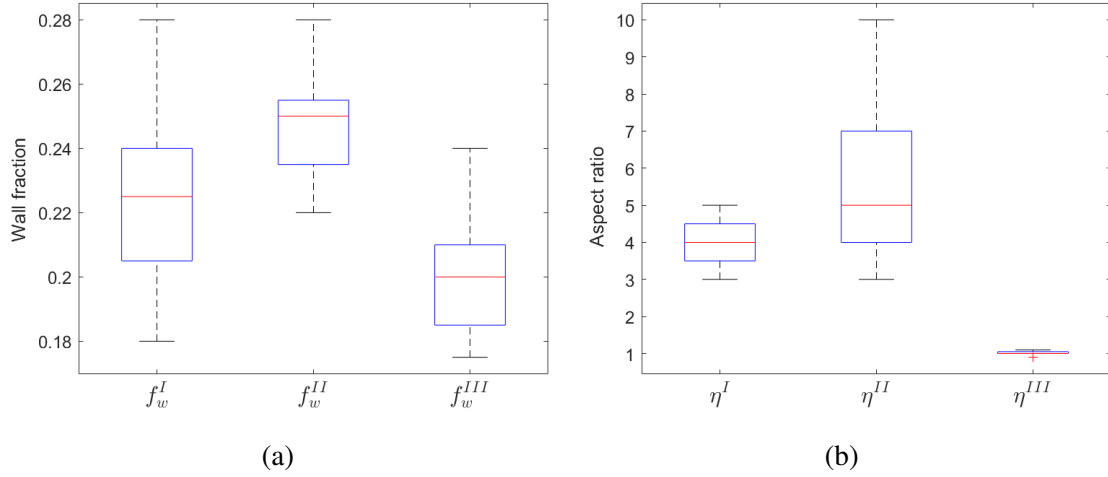


Figure 4.2: Characteristic mesoscale attributes a) Aspect ratio, η , and b) Wall fraction f_w , of each structure type computed from TEM images for Cu as explained on 4.1.4. In all cases, the plots correspond to a minimum of ten measurements.

stress strain curves for Cu single crystals, which are dominated by three characteristic dislocation activity, i.e, cross slip, Cottrell locks and Hirth locks. For each dislocation activity, a characteristic type of dislocation substructure exist: equiaxed cells for cross slip, semi-elongated cells for Cottrell locks and elongated cells for Hirth locks. The morphology of these structures can be directly quantified from TEM images. For example, η can be approximated as the ratio between the longest and shortest space in between walls while f_w can be computed as the ratio between the wall thickness and the wall spacing (Feaugas and coworkers [104]). Figure 4.4 demonstrates this methodology for equiaxed cell structures (Type III), i.e. $\eta^{III} \approx 1.0$ and $f_w^{III} \approx 0.2$. while Figure 4.5 and 4.6 demonstrate the estimations of dislocation structure attributes for semi-elongated cell (Type I) and elongated cell (Type II) structures, respectively. We have repeated this measurements in 12 images for Type III, [10–12, 16–18, 41], 15 images for Type I, [12, 15, 18, 41] and 9 images for Type II structures, [10, 18]. All the measurements done at least in 10 cells per image. We note that the TEM images were selected to represent well developed structures after significant amount of straining.

Table 4.3: Model mesoscale parameters used in the crystal plasticity model. All values are within the best independent guess from lower scale modelling and experiments.

Parameter	Experimental range	Optimized value
The self-interaction coefficient, A_{ii}	0.1 to 0.3	0.1 [42, 101]
The line tension, α_{LE}	0.5 to 1.5	1.0 [102, 103]
The dislocation multiplication factor, K_{multi}	1 to 4	1.0 [66, 102]
Similitude coefficient, K_{struct}	5 to 10	8 [70, 87]
Wall fraction - Type I, f_w^I	0.1 to 0.5	0.23
Wall fraction - Type II, f_w^{II}	0.1 to 0.5	0.25
Wall fraction - Type III, f_w^{III}	0.1 to 0.5	0.2
Aspect ratio - Type I, η^I	1.0 to 5.0	4.0
Aspect ratio - Type II, η^{II}	2.0 to 10.0	5.0
Aspect ratio - Type III, η^{III}	$\simeq 1.0$	1.0
Critical cross slip strain, γ_{Cr}	-	10^{-4}

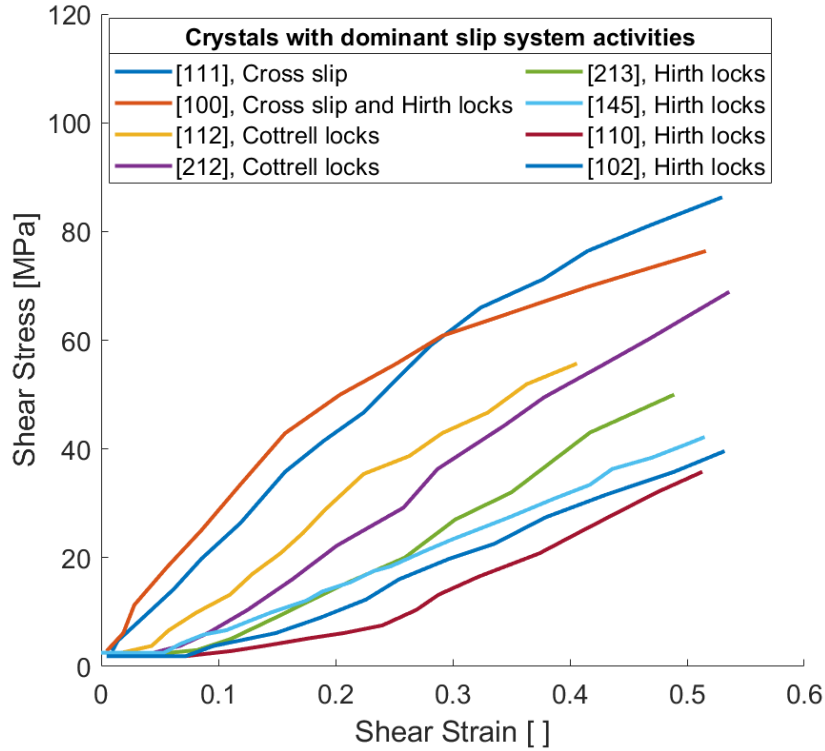


Figure 4.3: Experimental stress strain curves of Cu single crystals, three types of behavior are apparent. Each behavior type corresponds to a characteristic dominant dislocation activity, i.e, cross slip, Cottrell locks and Hirth locks (by performing a plasticity partitioning analysis, i.e, dividing the total strain by Schmid factor). For the crystals with two dislocation activity on the image, the first one is dominant. Although, for each dominant dislocation activity, a characteristic type of dislocation substructure exist from TEM images: equiaxed cells for cross slip, semi-elongated cells for Cottrell locks and elongated cells for Hirth locks.. The strain stress curves from [13–15].

100 Cu Crystal at 0.17 deformation, RT

Cell No.	Dislocation structure attributes			
	D (μm)	t (μm)	$f_w = t/D$	η
1	1.5	0.26	0.17	1.1
2	0.8	0.15	0.19	1.0
3	1	0.2	0.2	1.0
4	1	0.22	0.22	1.0
5	0.7	0.15	0.21	0.8
6	0.6	0.2	0.33	1.0
7	0.8	0.2	0.25	1.0
8	1.0	0.2	0.2	1.0
9	1	0.1	0.1	1.0
10	1.2	0.2	0.16	1.1
Average	0.96	0.19	0.2	1.0

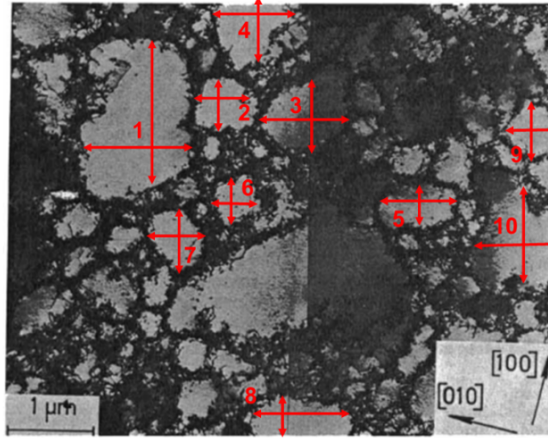


Figure 4.4: The TEM Cu dislocation substructure estimation strategy to estimate structure attributes for equiaxed cell structure (type III), i.e. $\eta^{III} \approx 1.0$ and $f_w^{III} \approx 0.2$. The values of cell size, aspect ratio and wall fraction measured in 10 cells and averaged. TEM image from [16].

112 Cu Crystal at 0.27 deformation, RT

Cell No.	Dislocation structure attributes			
	D (μm)	t (μm)	$f_w = t/D$	η
1	1.0	0.23	0.23	4.0
2	1.0	0.23	0.23	4.5
3	0.7	0.20	0.28	4.0
4	1.0	0.22	0.22	5.0
5	1.2	0.25	0.20	4.0
6	0.8	0.20	0.25	4.0
7	1.1	0.24	0.22	5.0
8	1.2	0.28	0.23	5.0
9	1.0	0.23	0.23	2.0
10	0.9	0.22	0.24	3.0
Average	0.99	0.23	0.23	4.0

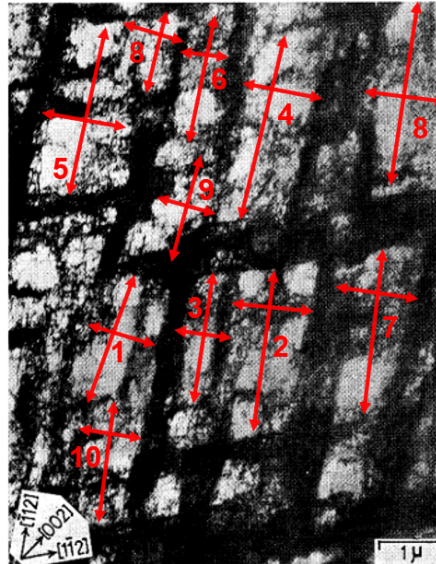


Figure 4.5: The TEM Cu dislocation substructure estimation strategy to estimate structure attributes for semi-elongated cell structure (type I), i.e. $\eta^I \approx 4.0$ and $f_w^I \approx 0.23$. The values of cell size, aspect ratio and wall fraction measured in 10 cells and averaged. TEM image from [15].

110 Cu Crystal at 0.27 deformation, RT

Cell No.	Dislocation structure attributes			
	D (μm)	t (μm)	$f_w = t/D$	η
1	0.8	0.22	0.28	5
2	0.8	0.27	0.34	5
3	0.9	0.22	0.24	4
4	1	0.21	0.21	5
5	1.2	0.25	0.21	5
6	0.9	0.22	0.24	6
7	0.8	0.21	0.26	5
Average	1.0	0.23	0.25	5.0

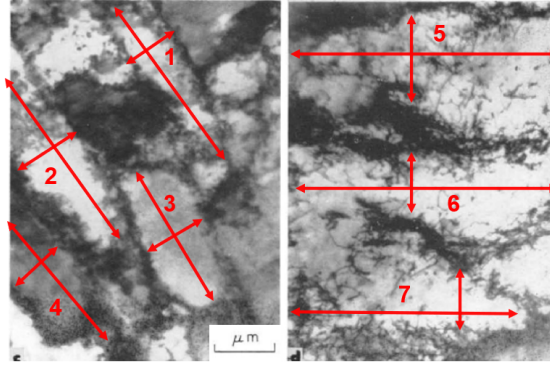


Figure 4.6: The TEM Cu dislocation substructure estimation strategy to estimate structure attributes for elongated cell structure (type II), i.e. $\eta^{II} \approx 5.0$ and $f_w^{II} \approx 0.25$. The values of cell size, aspect ratio and wall fraction measured in 7 cells and averaged. TEM image from [10].

4.1.5 Crystal/Grain Orientation Effect on Cross Slip and Cell Formation

Upon enough straining, cross slip will be activated and structures will evolve towards more equiaxed cell structures of Type III. For a fix applied strain, the critical cross slip strain, γ_{Cr} , controls the boundary that transitions into cells as shown by Figure 4.7. By decreasing γ_{Cr} , a larger fraction of the inverse pole figure develops cells.

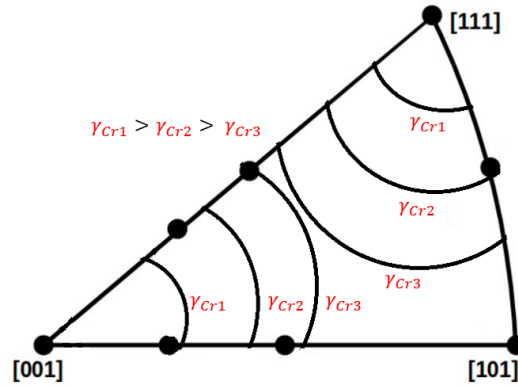


Figure 4.7: Schematic stereographic triangle representing the effect of γ_{Cr} on transitioning into Type III structures. The lines corresponds to the boundary that delimit the transition for various parameter values.

4.2 Finite Element Implementation and Results

The model was implemented on ABAQUS 2020 with a UMAT subroutine and a mesh with 8-node linear brick, reduced integration, and hourglass control elements (C3D8R) as shown in Figure 4.8. Polycrystalline representation corresponds to ten thousand random grain orientation distributions computed with MTEX [105]. We also did a mesh size analysis with various element (grain) numbers to assure enough refinement Figure 4.9.

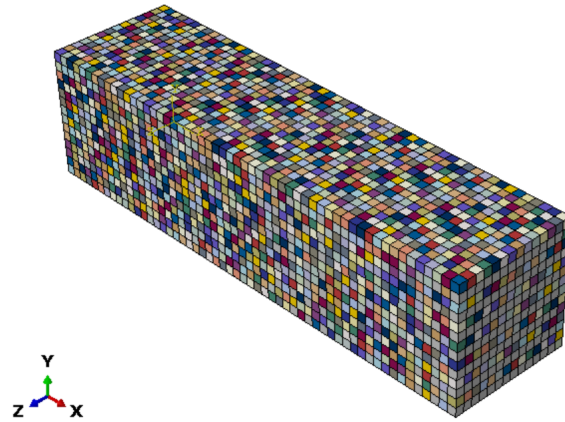


Figure 4.8: Specimen of $100 \times 100 \times 400$ mm dimension, used in finite element mesh with ten thousand elements and uniaxial boundary conditions. Pictorial description of different grains indicated with different colors (no correlation with Euler angles values).

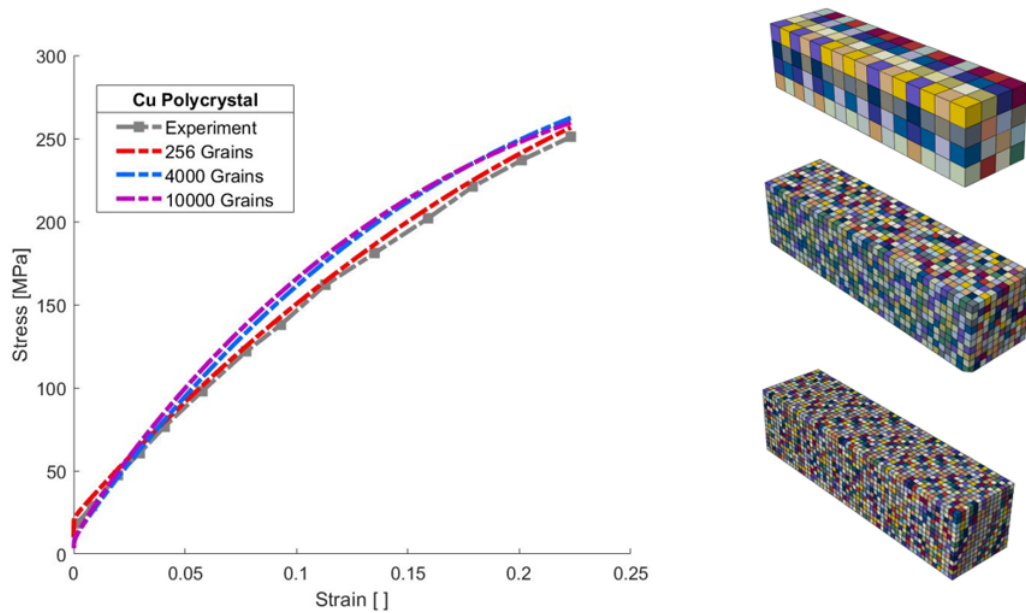


Figure 4.9: Mesh size analysis.

4.3 Monotonic Model Results

We first present the results for six Cu single crystals deformed under monotonic loading at a strain rate of 0.2 s^{-1} and 298K on Figure 4.10. The shear stress-strain curves was computing by using Schmid law. Compared to the experimental results from Takeuchi et al. [13], the model closely approximates stress-strain responses for all hardening stages. We highlight that these results validate the model from multiple orientations covering the three types of structures. Experimental true shear stress-true shear strain curves were obtained from true stress-true strain curves by Schmid factor ($\tau = M\sigma$, where M is Schmid factor) and true stresses-true strains were obtained from uniaxial tensile tests, [13]. Also, Predicted shear stress-shear strain curves were computed from predicted true stress-true strain curves by Schmid factor ($M_{111} = 0.27, M_{100} = 0.41, M_{110} = 0.41, M_{112} = 0.41, M_{212} = 0.41, M_{213} = 0.47$).

A key aspect for the robustness of the current model is the multiscale parameterization, which implies that the model can reproduce the macroscopic stress strain curves and also mesoscale attributes such as morphology, size and wall fraction. To validate this aspect, we evaluated TEM images at various strain levels and obtained ten measurements for the wall spacing, aspect ratio and wall fraction following the procedure on 4.1.4. Figure 4.11 compares the evolution of the wall spacing, wall fraction and aspect ratio of dislocation structures computed from models and experiments. Overall, the model reproduces qualitatively and quantitatively the general mesoscale response and supports the value of independent parameterization of dislocation structures for modeling crystal response.

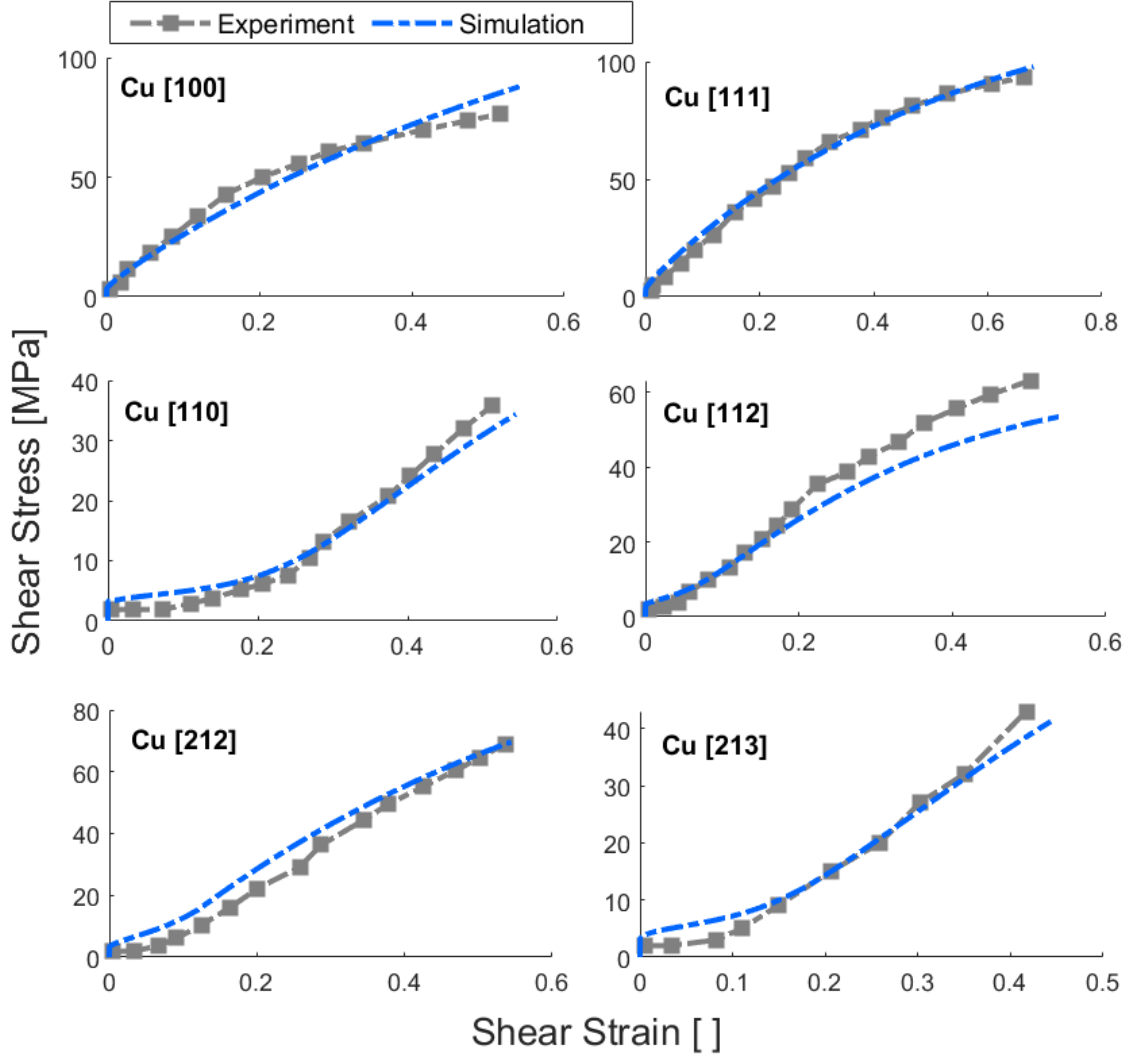


Figure 4.10: Comparison of the shear stress-shear strain curve of Cu single crystals from models and experiments. Experimental true shear stress-true shear strain curves were obtained from true stress-true strain curves by Schmid factor ($\tau = M\sigma$, where M is Schmid factor) and true stresses-true strains were obtained from uniaxial tensile tests, [13]. Also, Predicted shear stress-shear strain curves were computed from predicted true stress-true strain curves by Schmid factor ($M_{111} = 0.27, M_{100} = 0.41, M_{110} = 0.41, M_{112} = 0.41, M_{212} = 0.41, M_{213} = 0.47$). Experimental data taken from Ref. [13].

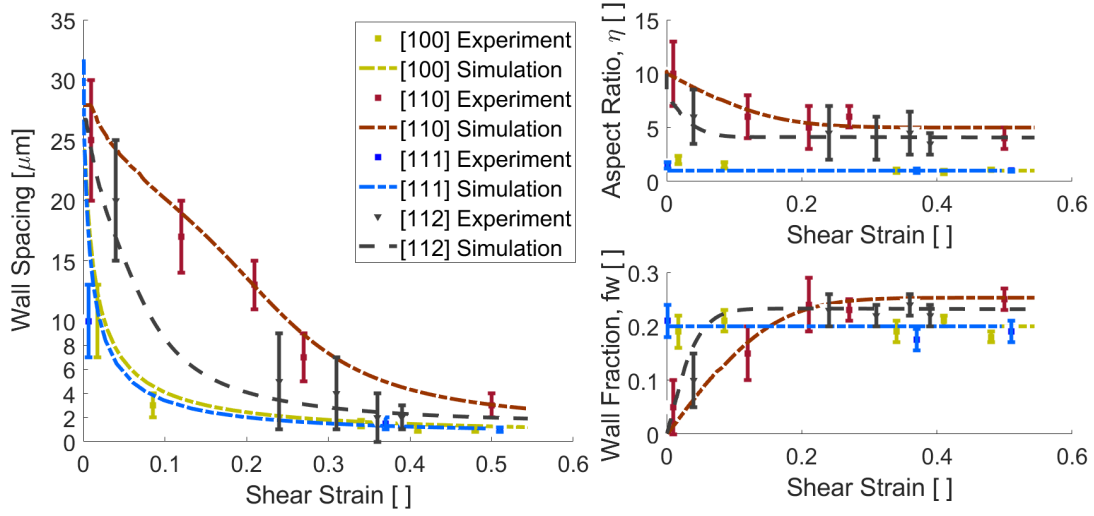


Figure 4.11: Mesoscale results of the model for Cu crystals. Experimental data taken from Ref. [11, 12, 16–18].

Given that mesoscale dislocation structures are common for FCC materials, we argue that our approach should be amenable to predict various material responses without adjusting mesoscale parameters. This property grant excellent predictive power to represent the response of single- and poly-crystals for other materials with similar mesoscale structures, even when single crystal data is not available, such as for austenitic stainless steel [106, 107] or high entropy alloys [108, 109]. Hence, we implemented the model for Ni at 298K and Al at 77K (0.1 to 0.2 homologous temperature) using identical mesoscale parameters. Figure 4.12 and Figure 4.13 present remarkable agreement considering that much of the hardening arising from dislocation structures was parameterized for Cu .

Since the single crystal model does not take into account crystal size effects, a fair comparison with polycrystals requires grain sizes large enough not to affect the the dislocation mean free path. Hence, we compare to experiments with large grains and limiting the maximum dislocation mean free path to the average grain size. The results for polycrystals in Figure 4.14 present excellent agreement between models and experiments. The model and the parameters are the same as those used for modeling single crystals, which reinforces the notion that matching single crystals provides good predictive power for polycrystals when grain size effects are not dominant. Figure 4.15 further presents the

equivalent the stress-strain response from each grain in the Cu simulation. Notably, the model results in significant variability among grains with the equivalent stress ranging from 60 MPa to 600 MPa at 20% deformation.

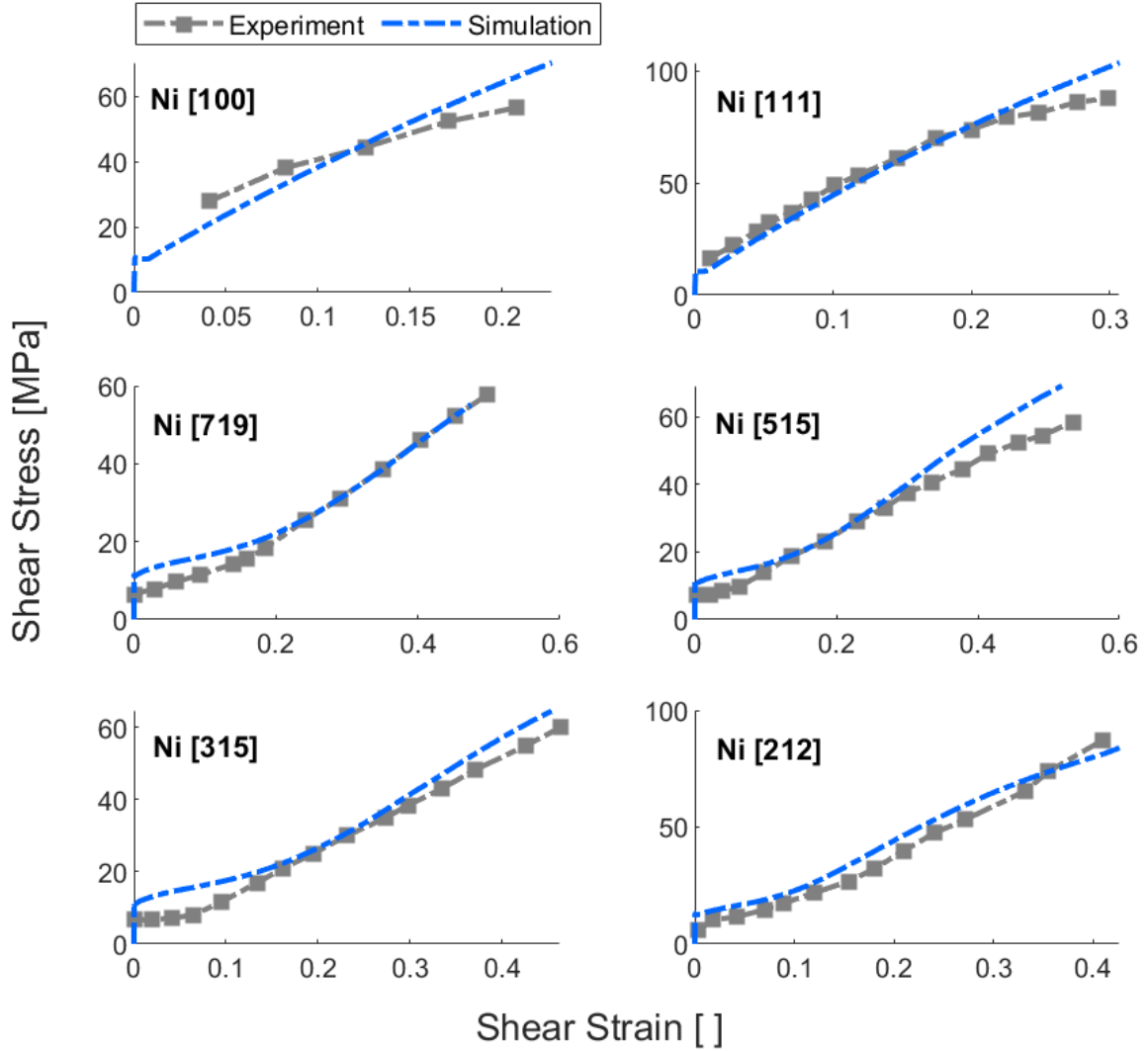


Figure 4.12: Comparison of the shear stress-shear strain curve of Ni single crystals from models and experiments. Experimental true shear stress-true shear strain curves were obtained from true stress-true strain curves by Schmid factor ($\tau = M\sigma$, where M is Schmid factor) and true stresses-true strains were obtained from uniaxial tensile tests, [19, 20]. Also, Predicted shear stress-shear strain curves were computed from predicted true stress-true strain curves by Schmid factor ($M_{111} = 0.27, M_{100} = 0.41, M_{719} = 0.47, M_{515} = 0.43, M_{315} = 0.49, M_{212} = 0.41$). Experimental data taken from Ref. [19, 20].

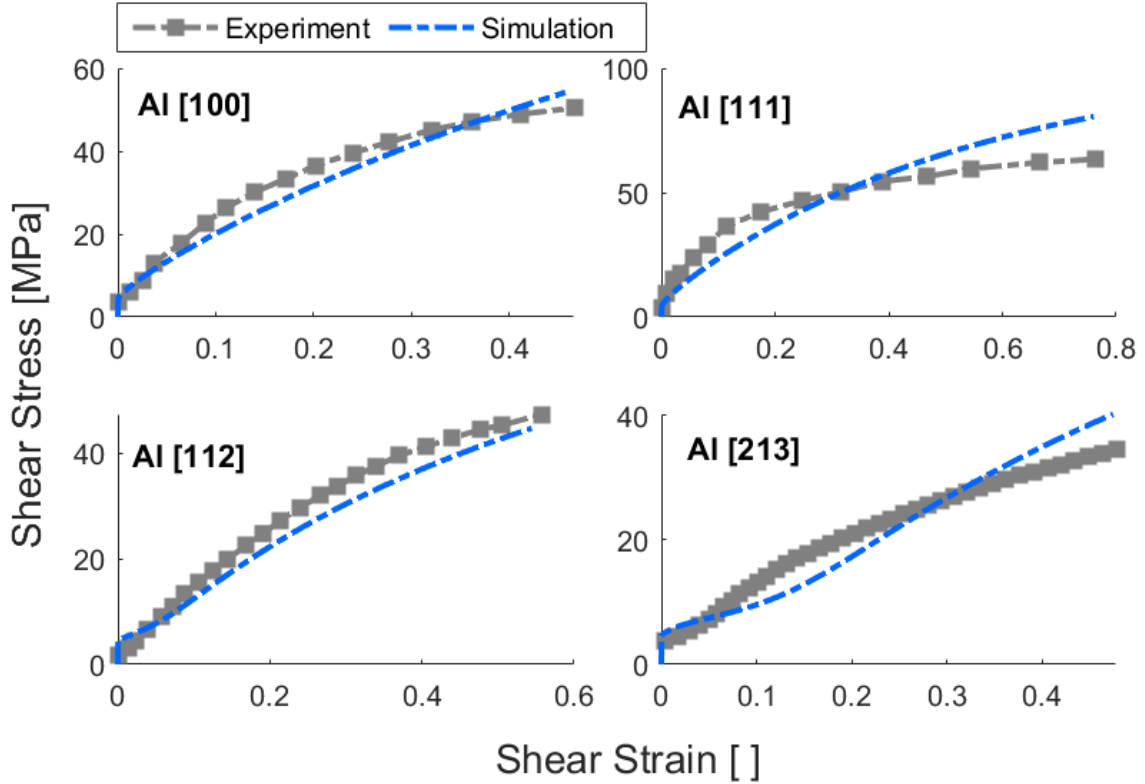


Figure 4.13: Comparison of the shear stress-shear strain curve of Al at 77K single crystals from models and experiments. Experimental true shear stress-true shear strain curves were obtained from true stress-true strain curves by Schmid factor ($\tau = M\sigma$, where M is Schmid factor) and true stresses-true strains were obtained from uniaxial tensile tests, [21, 22]. Also, Predicted shear stress-shear strain curves were computed from predicted true stress-true strain curves by Schmid factor ($M_{111} = 0.27, M_{100} = 0.41, M_{212} = 0.41, M_{213} = 0.47$). Experimental data taken from Ref. [21, 22].

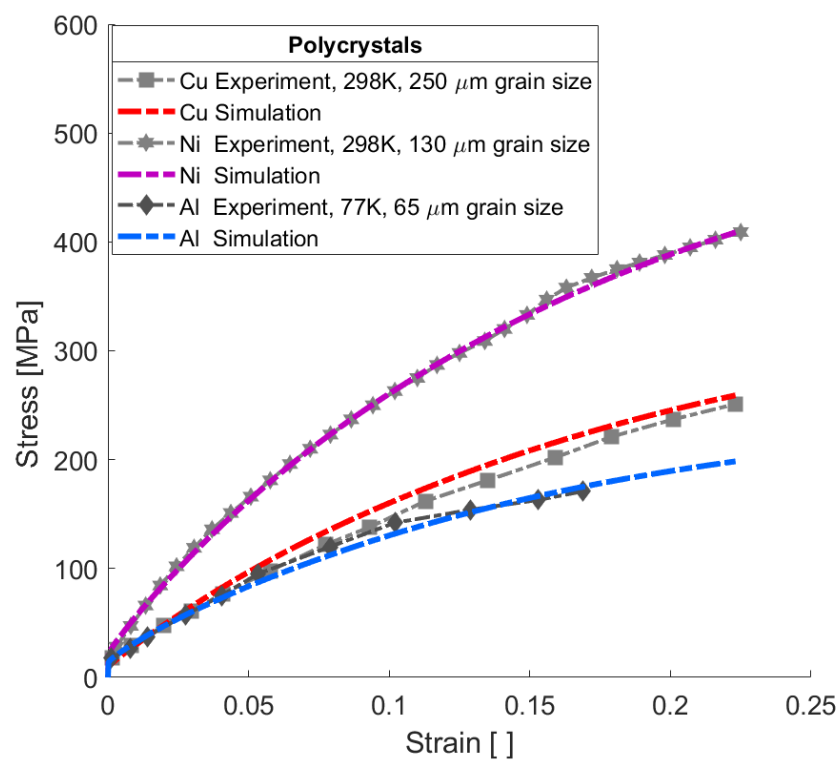


Figure 4.14: Simulation results for polycrystalline Cu, Ni and Al with the same unique set of model parameters as single crystals. Experimental data taken from Ref. [23–25].

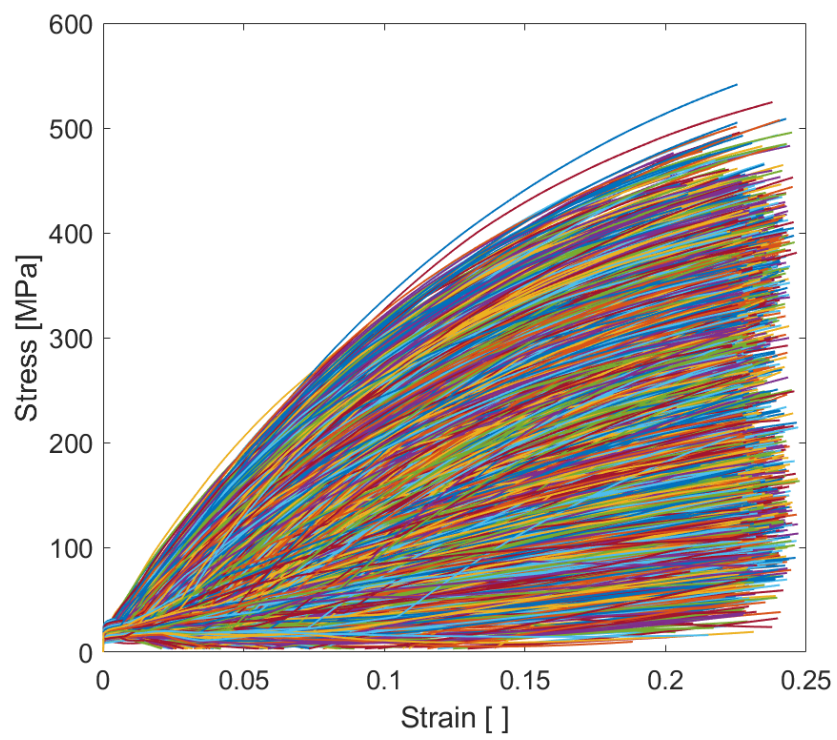


Figure 4.15: Equivalent stress-strain response from ten thousand grains from Cu polycrystal simulation.

4.4 Discussion

We have presented a crystal plasticity constitutive model that, for the first time, predicts the monotonic response of a large number of single crystal and polycrystals with a single model. The model relies on identifying mesoscale attributes by surveying the partition of plastic deformation among slip planes and can be applied to single and polycrystals indistinctly. The predictive power at the macroscopic scale is conferred by the independent validation of atomic- and meso-scale attributes.

By leveraging on TEM images and simulations we demonstrated that mesoscale parameters are identical (within the known certainty) among materials with similar structures. We have further quantified these *material-invariant* parameters (e.g., A_{ii} , f_w , η) confidently, which reduces the number of large uncertainty parameters. Hence, future applications of this crystal plasticity model should employ identical mesoscale parameters values along with an independent estimation of the atomic scale processes parameters (Table 4.2). We emphasize that pre-assumed low uncertainty parameters estimated independently in this work can yield better predictive results compared to the simultaneous fitting of multiple parameters using polycrystalline experimental data as shown next.

4.4.1 Lack of Predictive Power from Polycrystal Parameter Fitting

Several sets of parameters may predict the polycrystal behavior, but not all (if any) may reproduce single- and poly-crystal responses simultaneously. To exemplify this, we employed the mesoscale parameters on Table 4.4 to match the response of polycrystalline Cu (all other parameters still follow those on Table 4.1, Table 4.2, and Table 4.3). The three different sets of parameters result in good agreement between models and experiments as shown by Figure 4.16. However, when applied to single crystals, Figure 4.17 demonstrates that not all parameters are capable of predicting their responses. Notably, the error in predicting the stress reaches 100% for high Schmid factor crystals. Such large discrepancies at the crystal level demonstrate the limitations of parameterizations with

polycrystalline experiments and explains the limited success of those crystal plasticity models in predicting the local crystal response.

Table 4.4: Artificial sets of parameters recreated to show that one set may well predict polycrystals Cu but fail to predict single crystals. Other parameters were based on Table 4.1, Table 4.2 and Table 4.3.

Parameter	Set I	Set II	Set III
Wall fraction for Type II, f_w^{II}	0.25	0.2	0.1
Elongated structure aspect ratio for Type I, η^I	3.5	3.0	6.0
Similitude coefficient, K_{struct}	9.0	8.0	7.0

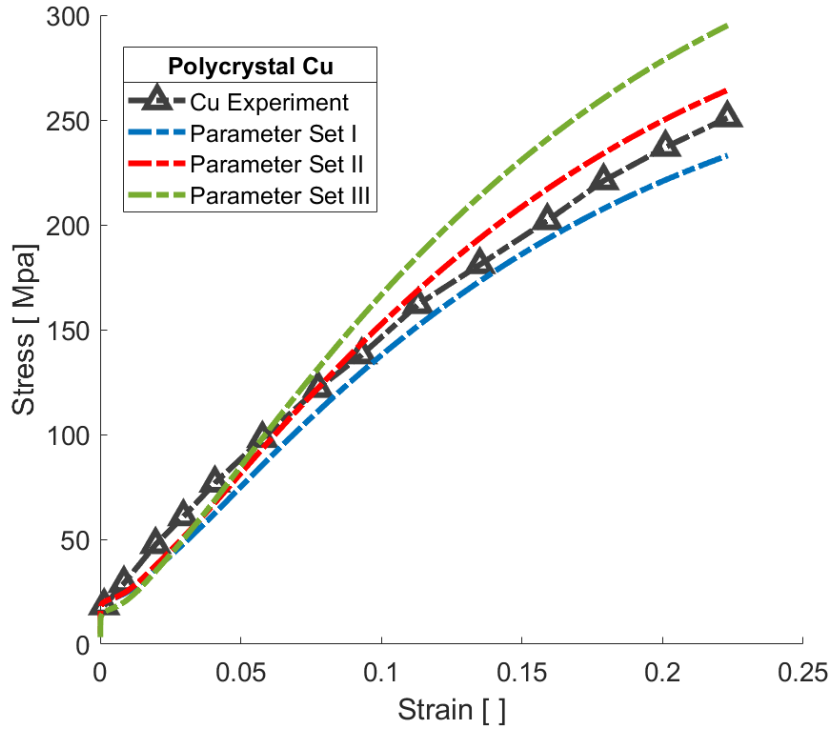


Figure 4.16: Results for polycrystalline Cu using different sets of parameters of Table 4.4. Acceptable agreement with experiment is achieved despite the differences on the parameters. The experimental data is taken from Ref. [24].

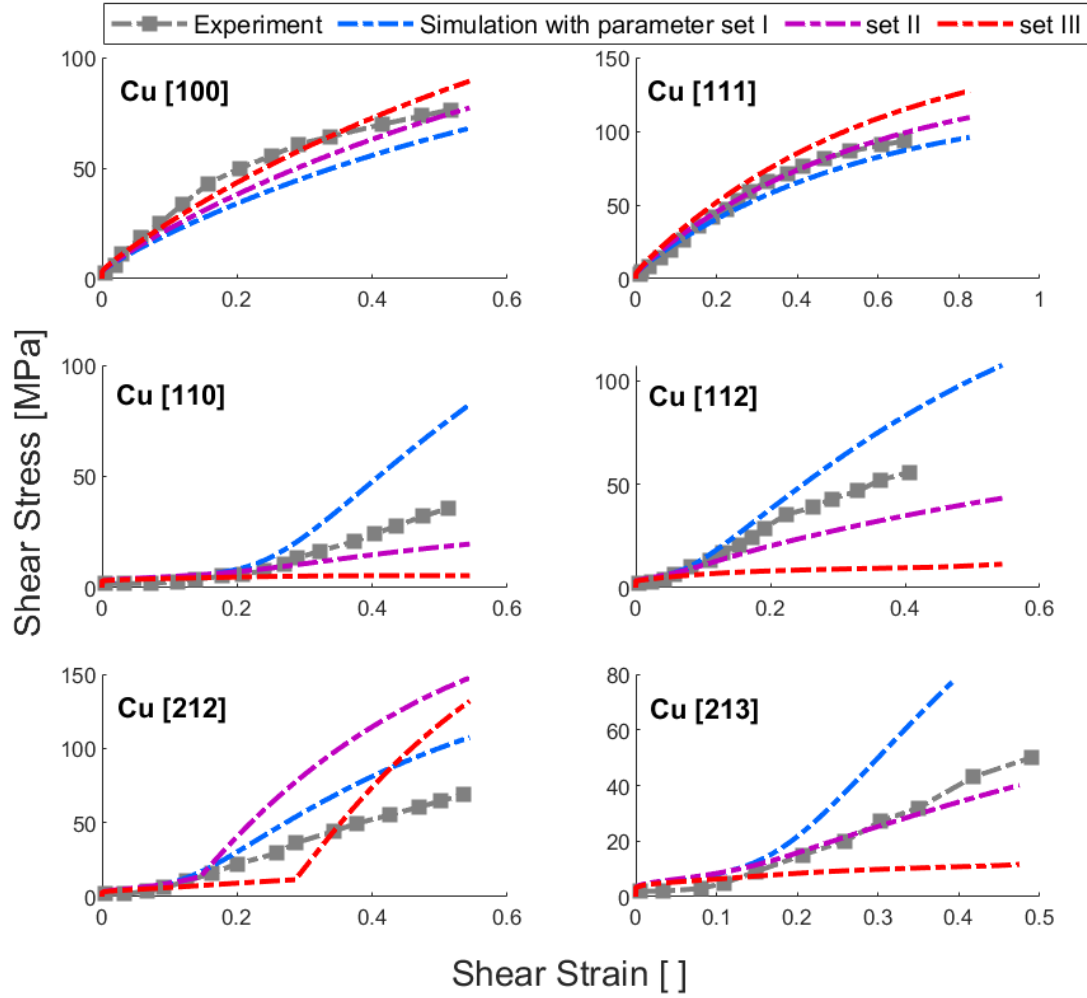


Figure 4.17: The shear stress-shear strain curve of Cu crystals with different artificial sets of parameters in Table 4.4. The sets of parameters predict polycrystal (Figure 4.16) but fail to predict single crystal responses. Experimental data is taken from Ref. [13].

4.4.2 Implications of Anisotropic Mean Free Paths

Next, we explore the role of the dislocation mean free path on the response of single crystals. Devincere et. al. [42] demonstrated with dislocation dynamics that the glide of dislocations is strongly anisotropic. Our approach indeed conveys this idea by assuming that the mean free path relates to the aspect ratio of each dislocation structure, which can be measured in experiments with relatively low uncertainty. A different and popular approach [80,110] relates the mean free path to the square root of the dislocation densities. For instance, Wang et. al. [111] computed the dislocation mean free path,

$$l_\alpha = \frac{1}{\sqrt{\alpha' \rho_\alpha}}, \quad (4.2)$$

with $\alpha' = 0.005$. We regard this formulation as harder to validate given the experimental uncertainty for quantifying dislocation densities. l_α was used instead of Equation (3.24) in Equation (3.22) to compute mobile dislocation density.

To understand the role of the mean free path anisotropy, we implemented two model variations using a constant aspect ratio [112] with $\eta = 1.4$ or Equation (4.2); All other aspects of the model remain the same as well as the same mesh and grain orientations used for polycrystalline simulations on Figures 4.14 and 4.15. Figure 4.18 confirms that both modifications still result in good agreement with the polycrystal experimental curve. However, Figure 4.19 demonstrates that both modifications cannot predict the single crystal responses. Indeed, a constant structure aspect ratio or Equation (4.2) result in fairly isotropic responses with all single crystals having almost the same response.

Figure 4.20 further presents the corresponding equivalent stress-strain curves for all 256 grains in the polycrystalline simulation. Compared to the results on Figure 4.15, the local variability in polycrystalline samples is drastically underpredicted when considering isotropic mean free paths ($\eta = 1.4$). These results further demonstrate that Equation 4.2 also underpredicts the glide anisotropy and has intrinsic limitations in predicting the local response. For identical polycrystalline samples, our mesoscale model predicts a maximum

equivalent stress 75% higher than those predicted with Equation (4.2). These miscalculations do not affect the average polycrystal response, but reduce the predictive power for single crystals and have important detrimental impact in damage prognosis. For example, the assessment of intergranular damage [113, 114] often requires the quantification of the local stress at grain boundaries, which can hardly be predicted with isotropic models. This scenario requires a mesoscale validation linked to the stress, which in our case is provided by the similitude principle and cannot be replaced by grain-level strain measurements.

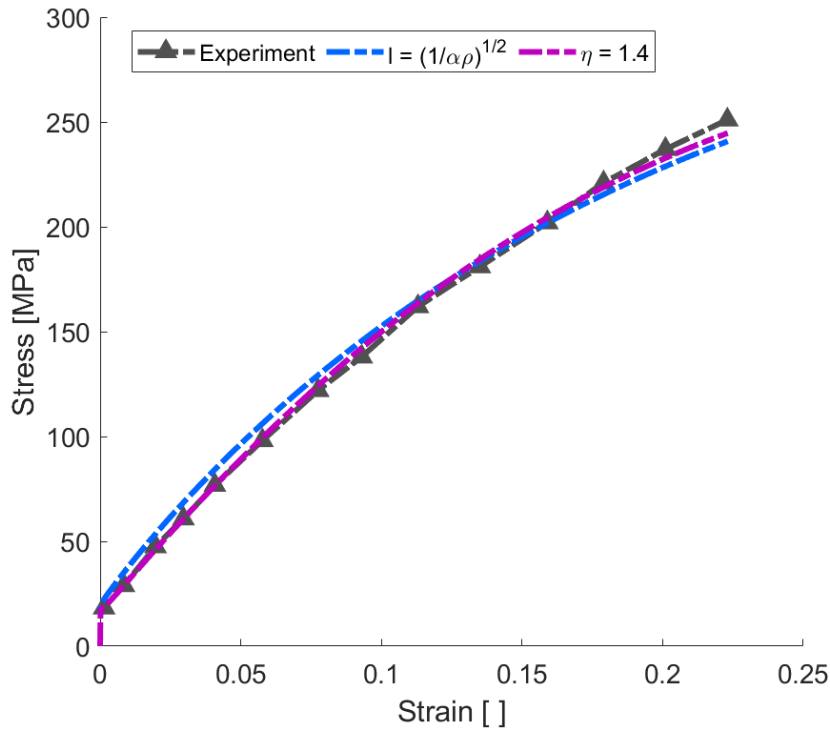


Figure 4.18: Polycrystalline Cu stress strain curves with $\eta=1.4$ ($l_{struc}=d_{struc}$) and Equation (4.2). The agreement of the model result with experiment shows that the models predict well polycrystals stress strain response. The experiment from [24].

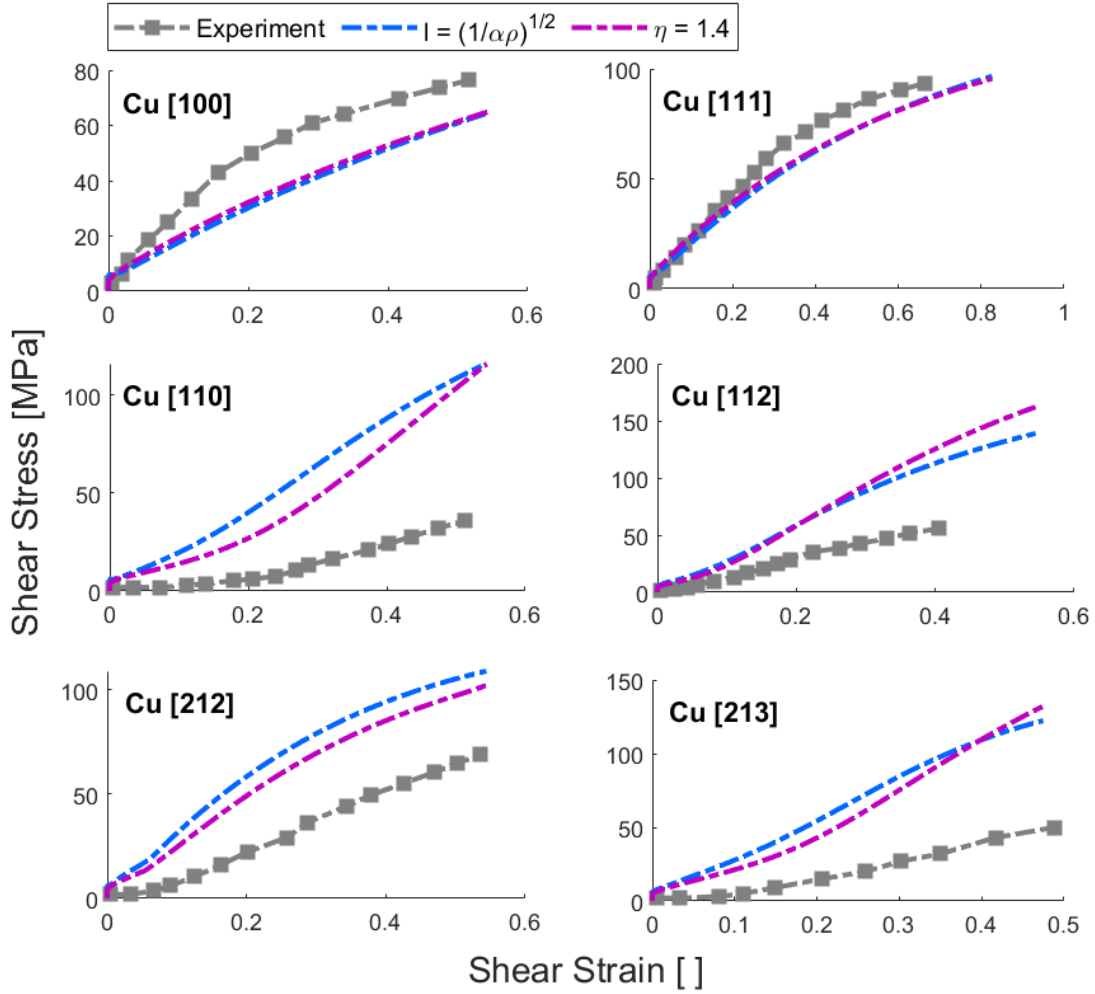


Figure 4.19: The shear stress-shear strain curve of Cu single crystals with isotropic dislocation mean free path ($l_{struc} = \eta d_{struc}$, $\eta=1.4$) and Equation (4.2). While these condition well predicts polycrystal, Figure 4.18, but fails to predict single crystals. The experiments from [13].

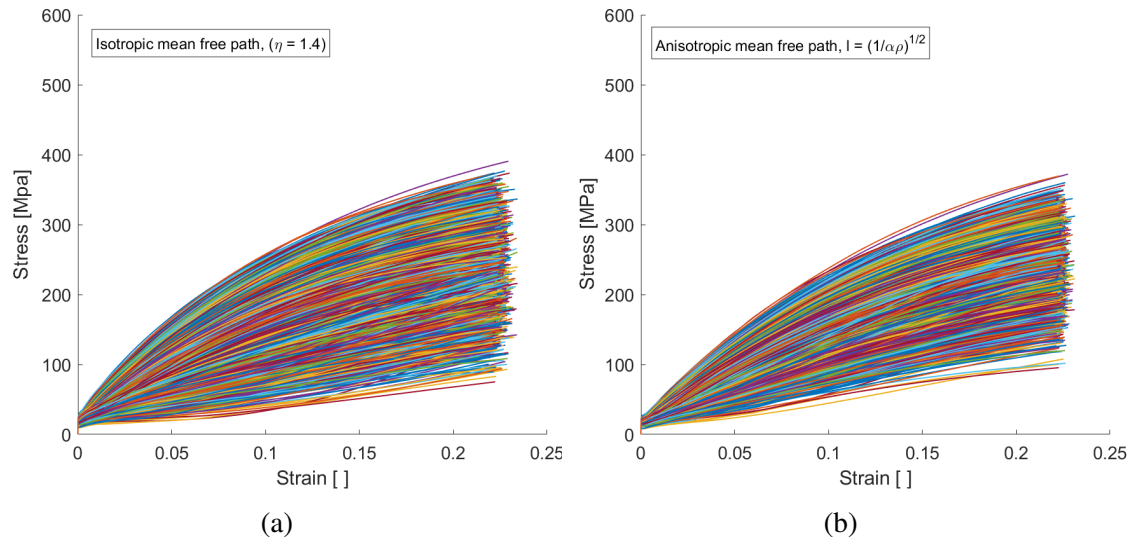


Figure 4.20: Grain-level equivalent stress-strain response for ten thousand grains in the polycrystalline Cu model using a) $\eta=1$ and b) Equation 4.2. Compared to Figure 4.15, the local variability is underpredicted by isotropic mean free paths models.

4.5 Summery of Equations

Macroscopic Cauchy stress, σ , 2nd Piola-Kirchhoff stress, σ^{PK2} , and Green strain tensor, $\mathbf{E}^e$, at current time increment, $t + \Delta t$ (t represents previous time step and $t + \Delta t$ corresponds to current new time step), are functions of elastic deformation gradient, $\mathbf{F}^e$,

$$\sigma_{t+\Delta t} = \frac{1}{\det(\mathbf{F}_{t+\Delta t}^e)} [\mathbf{F}_{t+\Delta t}^e \cdot \sigma_{t+\Delta t}^{PK2} \cdot (\mathbf{F}_{t+\Delta t}^e)^{-1}], \quad (4.3)$$

$$\sigma_{t+\Delta t}^{PK2} = \mathbf{C} : \mathbf{E}_{t+\Delta t}^e, \quad (4.4)$$

$$\mathbf{E}_{t+\Delta t}^e = \frac{1}{2} [(\mathbf{F}_{t+\Delta t}^e)^T \cdot \mathbf{F}_{t+\Delta t}^e - \mathbf{I}], \quad (4.5)$$

And elastic deformation gradient is being computed by decomposition of total deformation gradient to elastic and plastic part ($\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$).

$$\mathbf{F}_{t+\Delta t}^e = \mathbf{F}_{t+\Delta t} (\mathbf{F}_{t+\Delta t}^p)^{-1}, \quad (4.6)$$

where $\mathbf{F}_{t+\Delta t}$ is provided by Abaqus and $\mathbf{F}_{t+\Delta t}^p$ is being computed in the UMAT by velocity gradient, $\mathbf{L}_{t+\Delta t}$,

$$\mathbf{F}_{t+\Delta t}^p = \mathbf{L}_{t+\Delta t}^p \Delta t \mathbf{F}_t^p, \quad (4.7)$$

and the velocity gradient, $\mathbf{L}_{t+\Delta t}$, relates to local shear rates, $\dot{\gamma}^\alpha$,

$$\mathbf{L}_{t+\Delta t}^p = \sum_{\alpha=1}^{N_{sys}} \dot{\gamma}_{t+\Delta t}^\alpha (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha), \quad (4.8)$$

And local shear rates, $\dot{\gamma}_{t+\Delta t}^\alpha$, is being computed by solving the following constitutive equation,

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp \left(-\frac{F_0}{k_B T} \left\langle 1 - \left[\frac{\langle |\tau_{eff}^\alpha| \rangle}{s_t^0 \frac{\mu}{\mu_0}} \right]^p \right\rangle^q \right) \text{sgn}(\tau^\alpha - B^\alpha), \quad (4.9)$$

$$\tau_{eff}^\alpha = \langle |\tau^\alpha - B^\alpha| - S^\alpha \rangle, \quad (4.10)$$

$$\dot{B}^\alpha = \frac{f_w}{1 - f_w} \frac{2\mu(1 - 2S_{1212})}{1 + 4S_{1212}f_{Hill}^S} \dot{\gamma}^\alpha, \quad (4.11)$$

$$S^\alpha = \alpha_{LE} \frac{\mu b}{2d_{struct}} + \mu b \sqrt{A_{\alpha\beta} \rho^\alpha}, \quad (4.12)$$

$$\rho^\alpha = f(\dot{\gamma}^\alpha, l_{struct}, d_{struct}) \quad (4.13)$$

f_w , l_{struct} and d_{struct} are mesoscale structural parameters (walls fraction, dislocation mean free path and walls spacing, respectively) which are computed by mesoscale model as,

$$d_{struct} = K_{struct} \frac{\mu b}{\tau_{max}}, \quad (4.14)$$

$$l_{struct} = \eta d_{struct}, \quad (4.15)$$

$$f_w = f(\gamma, \gamma_{Max}, \gamma_{Cross}, \gamma_{Cottrell}, \gamma_{Hirth}), \quad (4.16)$$

$$\eta = f(\gamma, \gamma_{Max}, \gamma_{Cross}, \gamma_{Cottrell}, \gamma_{Hirth}), \quad (4.17)$$

More details of equations are represented in Figure 3.1 and 4.1.

4.6 Conclusions

This chapter introduced a physics-based crystal plasticity model based on mesoscale dislocation substructures that are observed in experiments. The model is designed so that all parameters and their uncertainty can be estimated independently from the macroscopic mechanical response, which enables multiscale validation. As a result, the model successfully predicts the monotonic mechanical response of single- and poly-crystals of FCC materials.

The model has been validated by comparing with the experimental stress strain curves from 16 single crystals and three polycrystals. In addition, the model correctly predicts the dominant dislocation substructures attributes (size, shape) as compared to those depicted by TEM images.

By characterizing mesoscale dislocation structures that are common for FCC materials, the approach can predict the mechanical response of various materials without modifying mesoscale parameters. This strategy grants a model excellent predictive power to represent the response of single- and poly-crystals for other materials with similar mesoscale structures, even when single crystal data is not available.

Finally, we demonstrated the importance of anisotropic mean free path formulations to predict the local response of single and polycrystals. We demonstrated that the models with more isotropic parameterizations of the mean free paths fail to predict single crystals and reduce the local variability, which is detrimental for damage prognosis.

Chapter 5

Sequential Physics-Based Crystal Plasticity Parameters Optimisation

5.1 Introduction

One significant drawback of crystal plasticity models is identification of large number of parameters with acceptable uncertainty. Parameter identification often relies on simultaneous fitting multiple parameters [75,110,115], which are non-unique and interdependent. Accordingly, several sets of parameters may be available and not all of these parameters (if any) are likely to reproduce single- and poly-crystal responses. For example Herrera-Solaz et al. [115] showed that different initial critical resolved stresses (CRSS) are reported in literature for Mg alloys by fitting experimental results on polycrystals. Different reported values are not reliable to be predictive in other conditions and an independent uncertainty analysis of parameters is needed.

Chapter 4 demonstrated that sets of parameters that match polycrystal stress-strain curves, do not guarantee good predictability of other crystals/orientations. Orientation dependency of the parameters requires more fundamental physical understanding to design parameter optimisation. Hence, this chapter presents a new physics based optimisation method to estimate the parameters with bounded uncertainty. Parameters are characteristic for each type of mechanisms and substructures in our model (Chapter 4). We limited applied strain range and loading direction to activate particular mechanisms and obtain specific substructure in which only one or two parameters are affected at a time. This strategy for different mechanisms and substructure enables us to estimate the parameters independently and reduce uncertainty. This approach relies on material invariant parameters which makes the proposed optimisation with one FCC material applicable for others with lack of experimental data.

5.2 Physics-Based Parameters Optimisation

Chapter 4 showed that equiaxed, elongated and semi-elongated cells are formed in loading condition (strain range and loading direction) with cross slip, Hirth and Cottrell locks activities, respectively. We designed a new optimisation sequence to estimate one sub-

structures parameters independent to others by controlling the loading condition. In the optimisation procedure, parameters at each sequential step are identified by fitting predicted and experimental stress strain curves. Optimised parameters are computed by minimizing the objective function,

$$f_{obj} = \sqrt{\sum_{i=1}^N \frac{(\sigma_i^{exp.} - \sigma_i^{sim.})^2}{(\sigma_i^{exp.})^2}}, \quad (5.1)$$

where $\sigma_i^{exp.}$ and $\sigma_i^{sim.}$ are experimental and predicted stresses at i_{th} strain level, and N is total number of experimental points. Incremental values of parameters during the optimisation are obtained in automated incrementation. Small values are added to parameters values, $(x + \delta x)$, at first increment, and the function value, f_1 is computed. Jacobian at next increment is being computed as,

$$J_n = \frac{f_{obj}^n - f_{obj}^{n-1}}{x^n - x_{n-1}}, \quad (5.2)$$

and the next values of the parameter are obtained,

$$x_{n+1} = x_n - \lambda \frac{f_{obj}^n}{J_n}, \quad (5.3)$$

where λ is a multiplier and n is Newton-Raphson iteration number. Notably, the parameters are limited in the experimental ranges described in Chapter 4. We argue that crystals and grains are large enough not to affect dislocation mean free path. Hence, we used large grain size experimental polycrystals in this work (250 μ in Cu, 130 μ in Ni, 65 μ in Al and 86 μ in stainless steel). The proposed optimisation is shown in Figure 5.1 and described in the following steps:

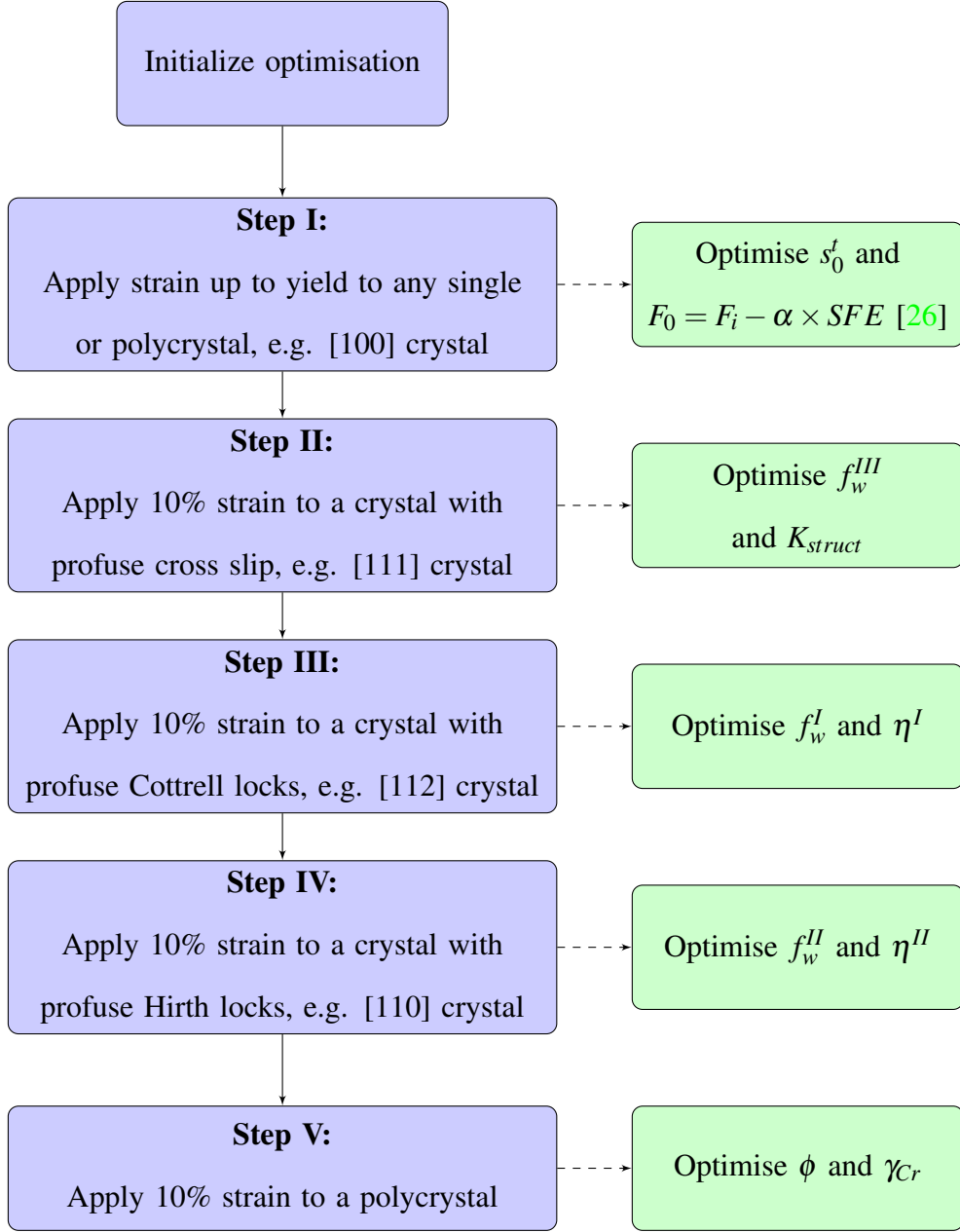


Figure 5.1: Sequential physics-based crystal plasticity parameters optimisation

5.2.1 Step I: Dislocation Glide Initiation (Yield)

Flow stress is minimum required stress for movement of dislocations. Dislocations need glide activation energy, F_0 and the thermal stress at 0 K, s_0^t , to surpass of obstacles. Ashraf and Castelluccio [26], showed that the glide activation energy, F_0 , correlate with the stacking fault energy in FCC metals and presented an equation to compute it. Numerous authors also reported 0-1 and 1-2 for p and q , respectively [63, 83, 116, 117]. Hence, s_0^t is

the only parameter that needs to be calibrated by any single or polycrystals flow stress (applied strain range needs to be limited up to yield), Figure 5.2.

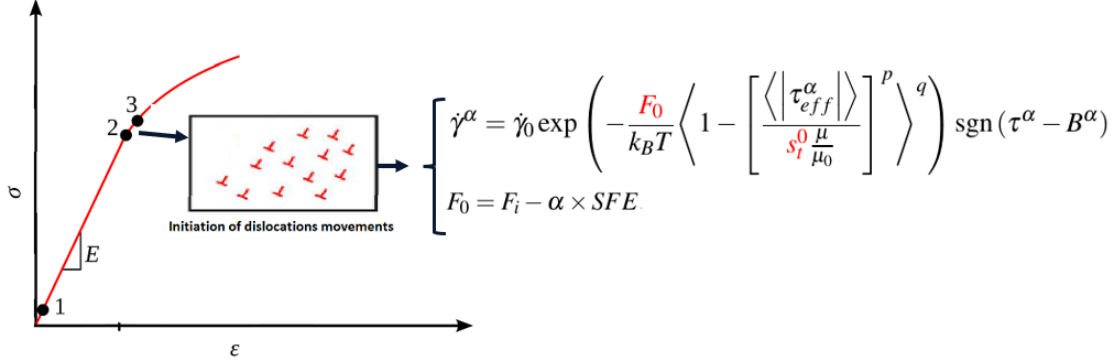


Figure 5.2: Physics-based calibration of glide activation energy, F_0 , and the thermal stress at 0 K, s_0^t . The F_0 is computed by equation, [26], and s_0^t is the only parameter that needs to be calibrated by any single or polycrystal flow stress. The calibrated parameters with flow stress, are shown in red in the equations.

5.2.2 Step II: Cross Slip and Equiaxed Cells

Equiaxed cells form only in crystals with profuse cross slip (e.g. [111] crystal). Change of equiaxed cells size (d_{struct}) with wall volume fraction of f_w^{III} , is the only structural change in the hardening stage II of these crystals. Accordingly, by limiting applied strain to this condition, we optimise f_w^{III} and similitude coefficient, K_{struct} , which are the only affecting parameters. Figure 5.3 represents the physics-based calibration of f_w^{III} and K_{struct} .

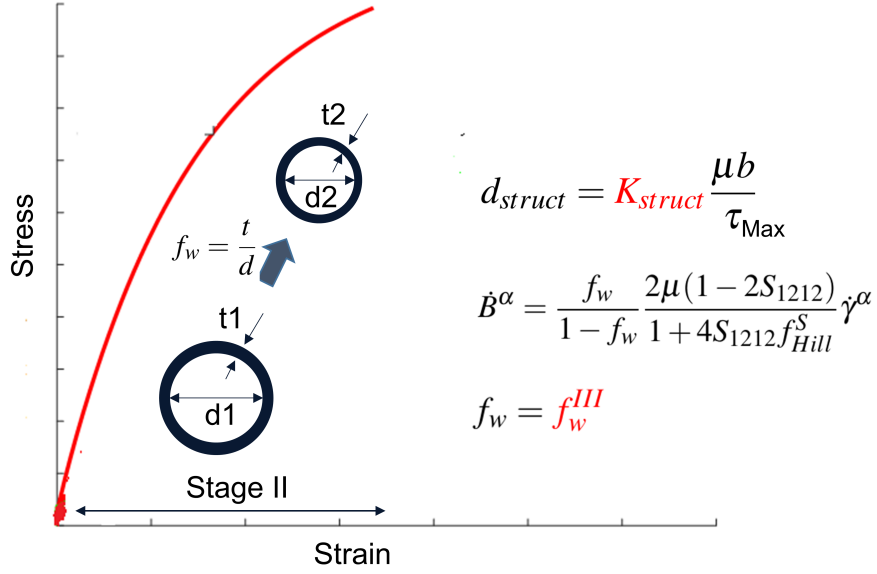


Figure 5.3: Physics-based calibration of equiaxed cells wall volume fraction, f_w^{III} , and similitude coefficient, K_{struct} , with cross slip dominated crystal. Cell size reduction is the only substructural change. f_w^{III} and K_{struct} , are the only affecting parameters at Stage II of crystals with profuse cross slip. Calibrated parameters with cross slip crystals. i.e. [111], are shown in red in the equations.

5.2.3 Step III and IV: Hirth and Cottrell Locks and Elongated Cells

Elongated cells develop in single slip crystals with Hirth Locks dominated slip systems and without cross slip. Change of wall volume fraction, f_w^{II} , aspect ratio, η^{II} , and wall spacing, d_{struct} , of elongated cells are structural changes in these crystals. The parameter controls the wall spacing, (K_{struct}), is calibrated in the previous section. Consequently, f_w^{II} and η^{II} are calibrated by these crystals, as shown in Figure 5.4. Same as Hirth locks, wall fraction, f_w^I and the aspect ratio, η^I , of semi-elongated cells are calibrated with a crystal with dominant Cottrell locks slip system.

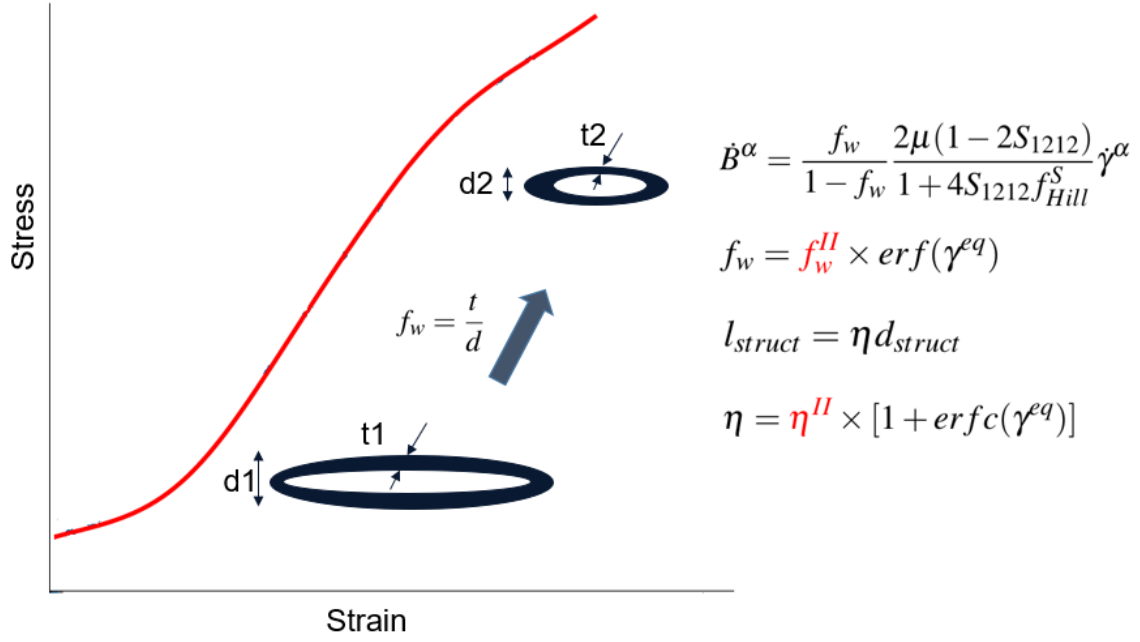


Figure 5.4: Physics-based calibration of wall volume fraction, f_w^{II} and the aspect ratio, η^{II} of elongated cells with Hirth locks dominated crystal (without cross slip). K_{struct} is calibrated in the previous section. Calibrated parameters with Hirth locks dominated crystals. i.e. [110], are shown in red in the equations.

5.2.4 Step V: Critical Cross Slip Strain and Equiaxed Cell

Chapter 4 showed that, for a fixed applied strain, critical cross slip strain, γ_{cr} , controls boundary of transitions into cells. Hence, the γ_{cr} is calibrated from polycrystal experimental data to capture the transition of enough grains to equiaxed cells. Also, cross slip efficiency, ϕ , controls the annihilation and production of dislocation density in polycrystals.

5.3 The Advantages of the Proposed Optimisation Method

5.3.1 Experimental Data Variability and Availability

Optimised parameters that use a single stress-strain curve from polycrystal do not guarantee to be predictive for other orientations. Accordingly, optimisation with more data enables higher quality prediction. Figure 5.5a and 5.5b show optimisation of parameters f_w^{III} and K_{struct} with one ([110] crystal]) and two stress strain curves ([100] and [110] crystals) of copper crystals (other parameters based on Chapter 4). Optimised parameters with one and two curves are named Set-I and Set-II, respectively, and are shown in Figure 5.5. Figure 5.5c represents the predictions of [111] copper crystal with Set-I and Set-II parameters. Blue and red curves in Figure 5.5c are predictions with Set-I and Set-II parameters, respectively. Since the red curve is closer to experimental curve, parameters optimised with two data give better predictive power. However, more data are not always available and running experiments are sometimes expensive, time consuming and difficult. This data shortage limits the predictability of crystal plasticity models and demands parameters optimisation methods that need fewer data and saved prediction quality.

5.3.2 Parameters Uncertainty

Evaluation of parameter uncertainty is a key aspect in crystal plasticity models predictability. Known physical sources of parameters in the proposed optimisation enable independent estimation of parameter uncertainty. For instance, f_w^{II} is wall fraction of Elongated Cells and has values 0.22-0.28 from the measurements of TEM images (Figure 4.2). Values outside this range (i.e. $f_w^{II} = 0.1$) fail to predict the crystals with Elongated Cell structure, i.e. [719] in Figure 5.6a, (other parameters based on Chapter 4). Predicting of [111] crystal in Figure 5.6a with $f_w^{II} = 0.1$ shows that capturing of experimental curves does not imply acceptable uncertainty of parameters and an independent estimation is needed. Figure 5.6b represents prediction of Ni [111] and [515] crystals with $f_w^{II} = 0.25$ which is in the experimental range and has low error. Contrary to Figure 5.6a, very good

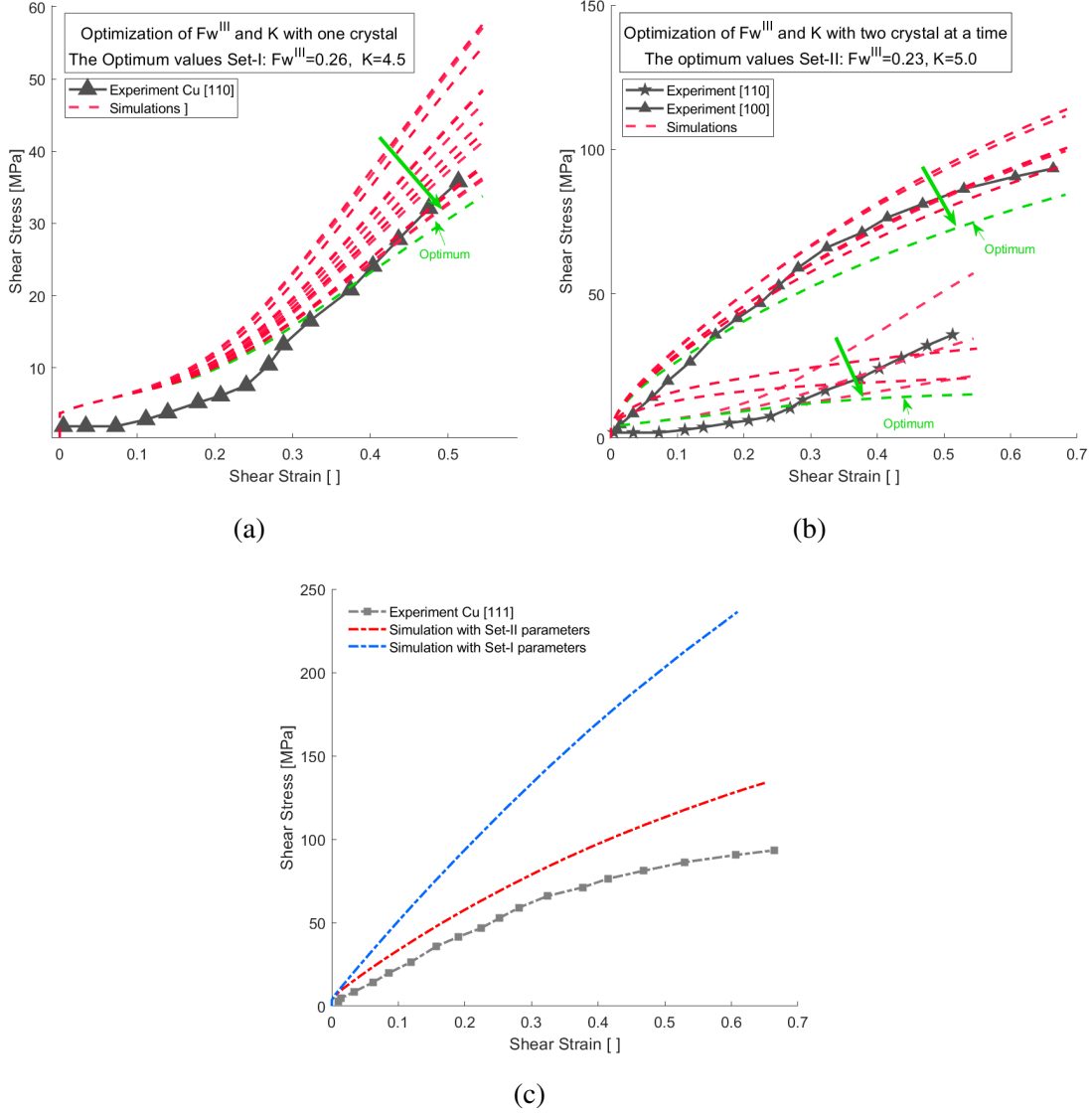


Figure 5.5: Optimisation of parameters f_w^{III} and K_{struct} with a) One ([110] crystal) and b) Two stress strain curves ([100] and [110] crystals) of copper crystals. Optimised parameters are Set-I and Set-II respectively. c) Predictions of [111] copper crystal with Set-I and Set-II parameters. Parameters optimised with two data give better predictive power. However, more data are not always available and running experiments are sometimes expensive, time consuming and difficult. This data shortage limits predictability of crystal plasticity models and demands parameters optimisation methods that need fewer data and saved prediction quality. Red curves are predictions with not-optimised parameters and show the optimisation path. Experiments from Ref. [13].

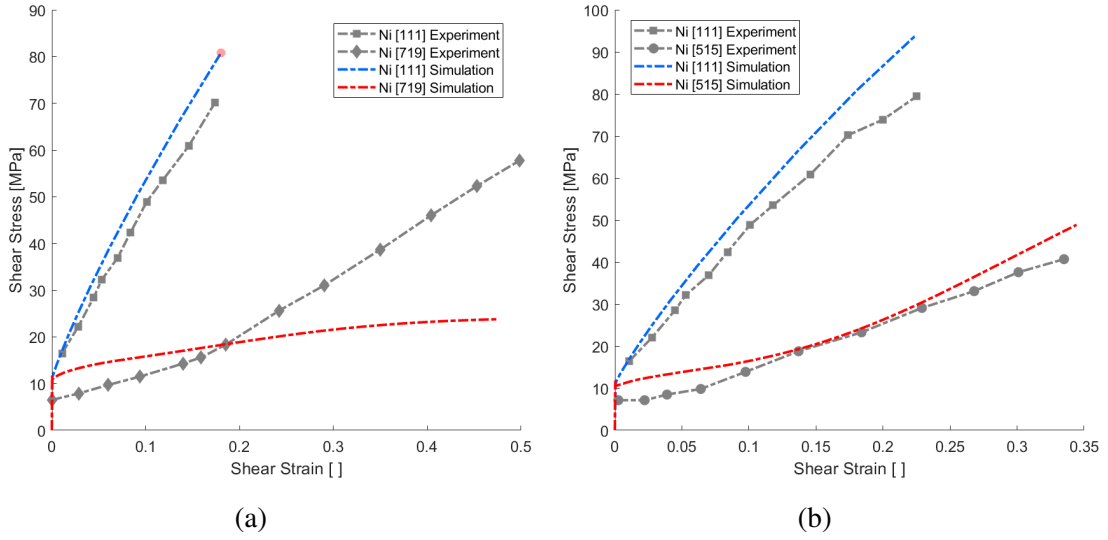


Figure 5.6: Known physical sources of the parameters in the proposed optimisation enable independent estimation of parameters uncertainty. For instance, f_w^{II} is wall fraction of Elongated Cells and has values 0.22-0.28 from the measurements of TEM images (Figure 4.2). a) Values outside this range (i.e. $f_w^{II} = 0.1$) fail to predict the crystals with Elongated Cell structure, i.e. [719]. Predicting of [111] crystal with $f_w^{II} = 0.1$ shows that capturing experimental curves does not imply acceptable uncertainty of parameters and an independent estimation is needed. b) Prediction of Ni [111] and [515] crystals with $f_w^{II} = 0.25$ which is in the experimental range and has low uncertainty. Contrary to a, very good agreements with experiments in both cases are apparent in b. Red curves are predictions with not-optimised parameters. Experiments from Ref. [19,20].

agreements with experiments in both cases are apparent.

5.3.3 Fitting Quality with Single and Multi Objective Function

Several authors used multi objective functions to optimise crystal plasticity parameters simultaneously [75, 79, 110]. Hence, optimisation with one curve at a time, i.e. single objective function, is being used in each step of the proposed sequential optimisation method (Figure 5.1). Figure 5.5a and 5.5b show that optimisation with one curve gives better fitting quality. For example, f_w^I is wall fraction of Semi-Equiaxed Cell structure that forms in crystals with Cottrell dominated slip activity (eg, [112] crystal). Hence, only [112] crystal is enough to optimise f_w^I . Figure 5.7 shows the optimization of f_w^I with excellent fitting quality.

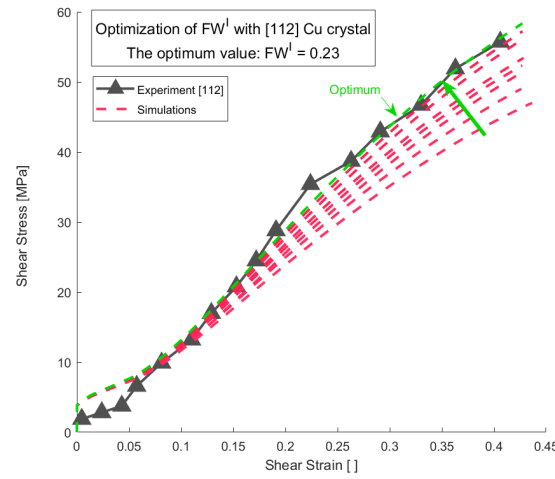


Figure 5.7: Excellent fitting quality of optimisation of f_w^I . Compared with Figure 5.5b in which the optimisation has been done with multi objective function, fitting quality is higher here. Since parameters are calibrated within limited physics in our model (Chapter 4), the optimisation can be done with single objective function with high fitting quality. Red curves are predictions with not-optimised parameters and show the optimisation path. Experiments from Ref. [13].

5.4 Application to Cu, Ni and Al

Optimisation of model parameters for Cu, Al and Ni are shown in Figures 5.8, 5.9 and 5.10, respectively. Notably, since experimental data required for optimisation stage IV of Al and stage III of Ni are missing, material invariant parameters (f_w^H for Al and f_w^L for Ni) of these steps were chosen from Cu data. Green lines are the predictions with optimised parameters resulting in better predictions compared to Chapter 4.

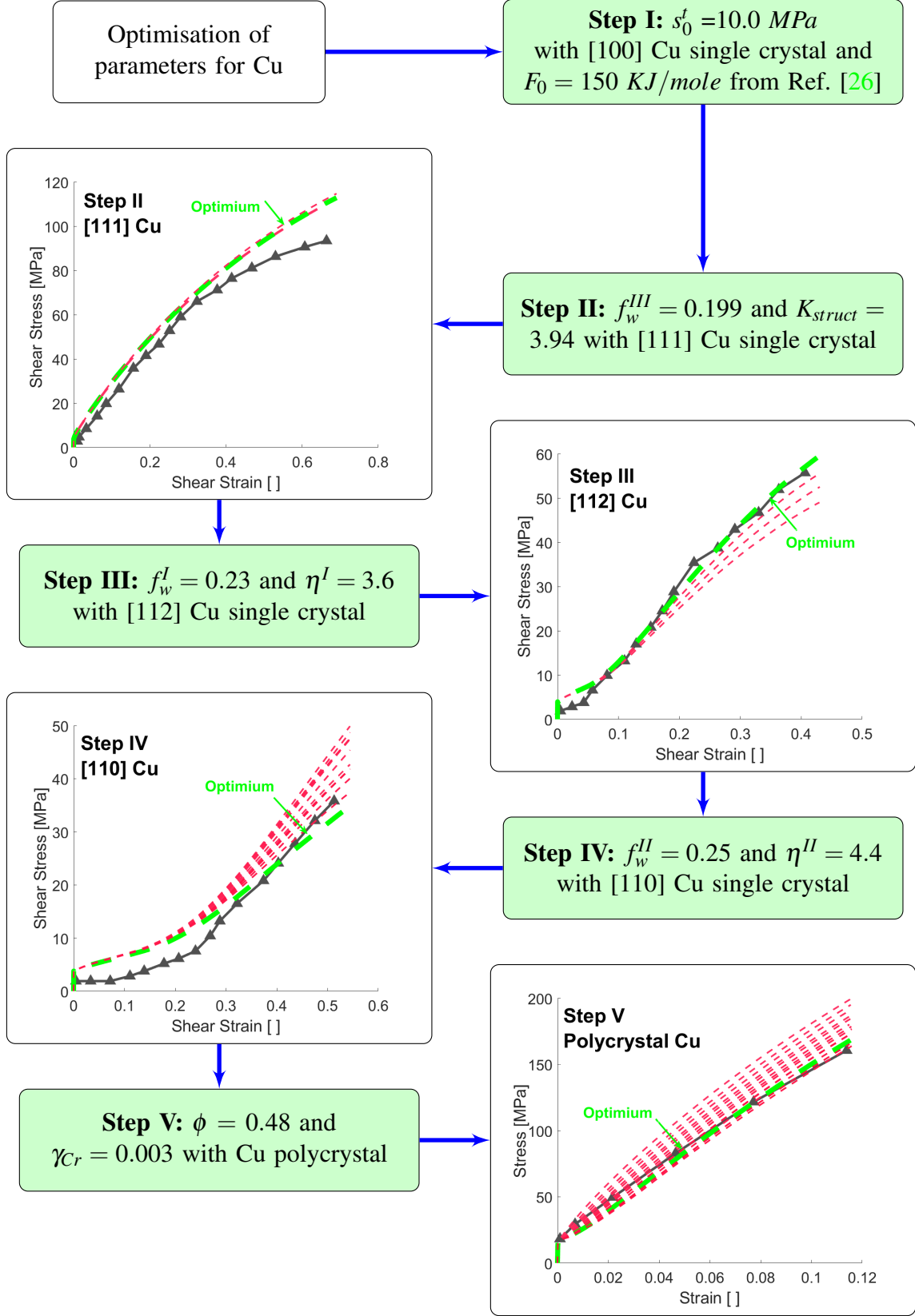


Figure 5.8: Sequential physics-based parameter optimisation for Cu. Green lines are predictions with optimised parameters. Better predictions are apparent compared to Figures 4.10. Red curves are predictions with not-optimised parameters and show the optimisation path. Gray points experimental data taken from Ref. [13].

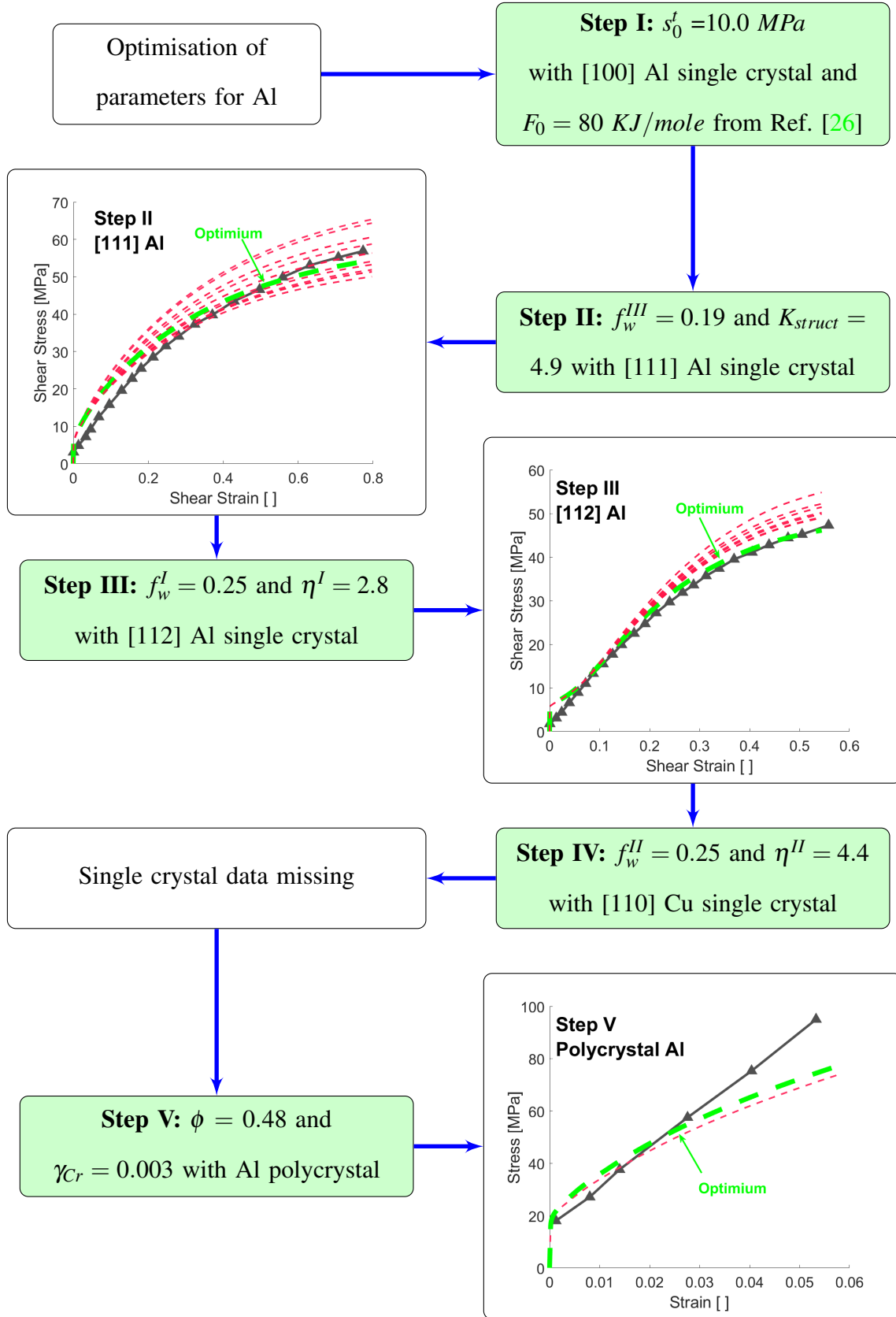


Figure 5.9: Sequential physics-based parameter optimisation for Al at 77 K. Green lines are predictions with optimised parameters. Better predictions are apparent compared to Figures 4.13. Red curves are predictions with not-optimised parameters and show the optimisation path. Gray points Experimental data taken from Ref. [21, 22].

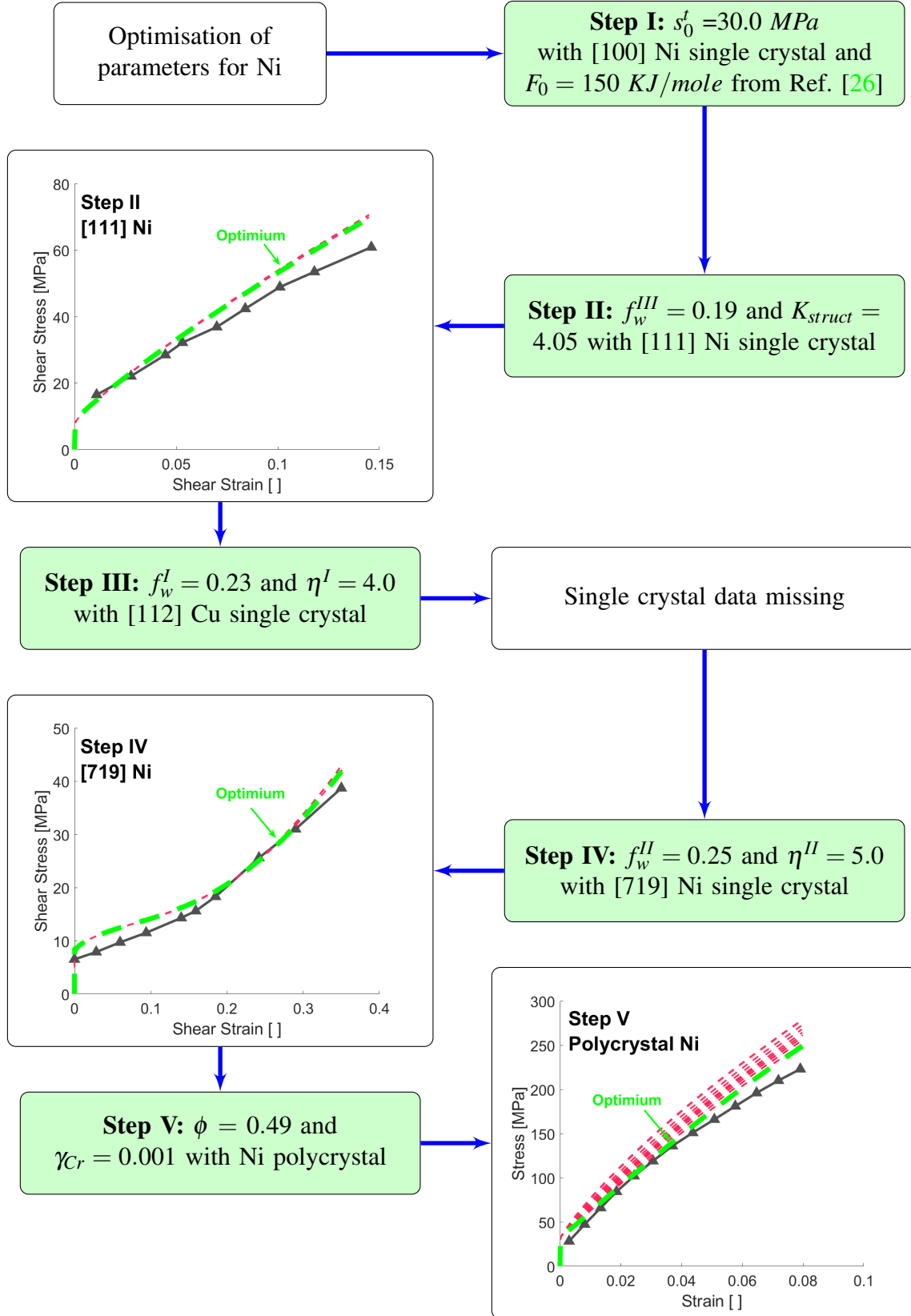


Figure 5.10: Sequential physics-based parameter optimisation for Ni. Green lines are predictions with optimised parameters. Better predictions are apparent compared to Figures 4.12. Red curves are predictions with not-optimised parameters and show the optimisation path. Gray points Experimental data taken from Ref. [19,20].

5.5 Discussion

To compare prediction power of the simultaneous optimisation of the parameters and the novel proposed optimization, we applied both methods to compute model parameters for stainless steel (316L). Parameters optimized by fitting to polycrystal data (conventional optimization) are listed in Table 5.1 and predictions of stress strain curves with those parameters are shown in Figure 5.11. Experimental stainless steel single crystals were grown with the Bridgman technique and were then homogenized for 30 h at 1470 K [27]. We used the same finite element geometry, mesh, and boundary condition explained in Chapter 4 (Figure 4.8) in stainless steel predictions. Single and polycrystal experimental data are from two sources with different chemical compositions which affects the s_0^t (250 MPa for single and 180 MPa for poly-crystal). While parameters predict well polycrystal behaviour, they fail to predict single crystals, which shows that optimization with polycrystal data fitting can not guarantee the predictability of single crystals.

Table 5.1: Parameters optimized by conventional methods by fitting with polycrystal data (other parameters were based on chapter 4).

Parameter	Optimized value (polycrystal fitting)
Thermal stress at 0 K , s_0^t , MPa	205 (single), 180 (poly-crystal)
Wall fraction for Type I , f_w^I	0.3
Wall fraction for Type II , f_w^{II}	0.3
Wall fraction for Type III , f_w^{III}	0.1
Elongated structure aspect ratio for Type I , η^I	5.0
Similitude coefficient, K_{struct}	6.0

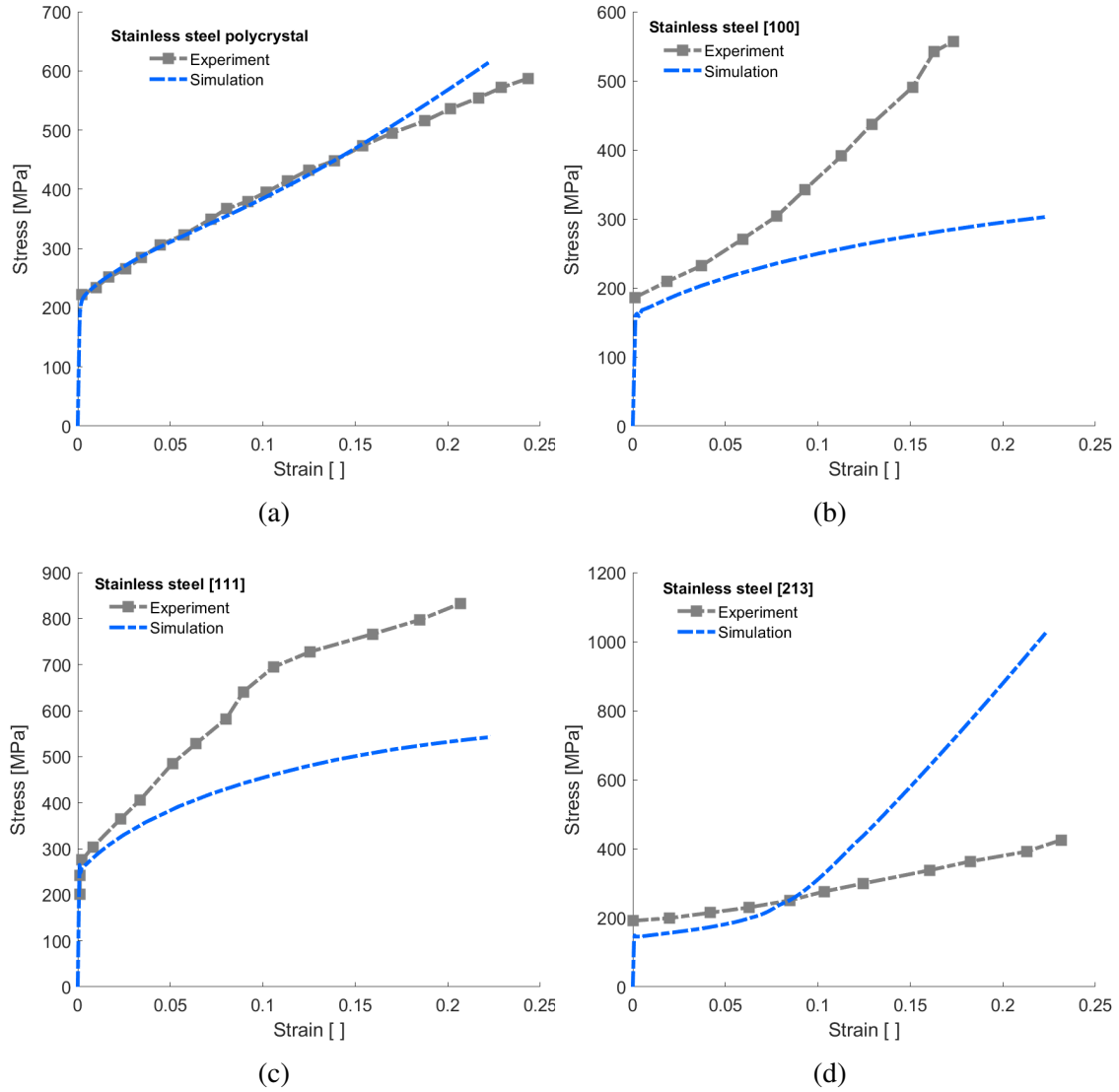


Figure 5.11: Prediction of stress strain curves of stainless steel (316) at 293 K from applying conventional optimization by fitting with polycrystal. While parameters predict well polycrystal, fail to predict single crystals, which shows that optimization with polycrystal data fitting can not guarantee predictability of single crystals. Experiments from Ref [27,28].

Now, we apply the proposed optimisation to calibrate parameters for stainless steel and results are shown in Figure 5.12. Chapter 4 showed that mesoscale parameters are material and orientation invariant, which enables us to blindly predict behaviour of new materials and orientations. Hence we applied the proposed optimization method to predict stainless steel behaviour with experimental data of other FCC materials, i.e Cu, Ni and Al. parameters. Optimized parameters by proposed method for Cu, Al, Ni and stain-

less steel are summarized in Table 5.2. Figure 5.13 presents prediction of stainless steel stress strain curves with parameters optimised separately by Cu, Ni, Al and stainless steel experimental data. While the other materials parameters predict the general trend with better predictions compared to other optimisation methods, Figure 5.11, but the results can be further improved.

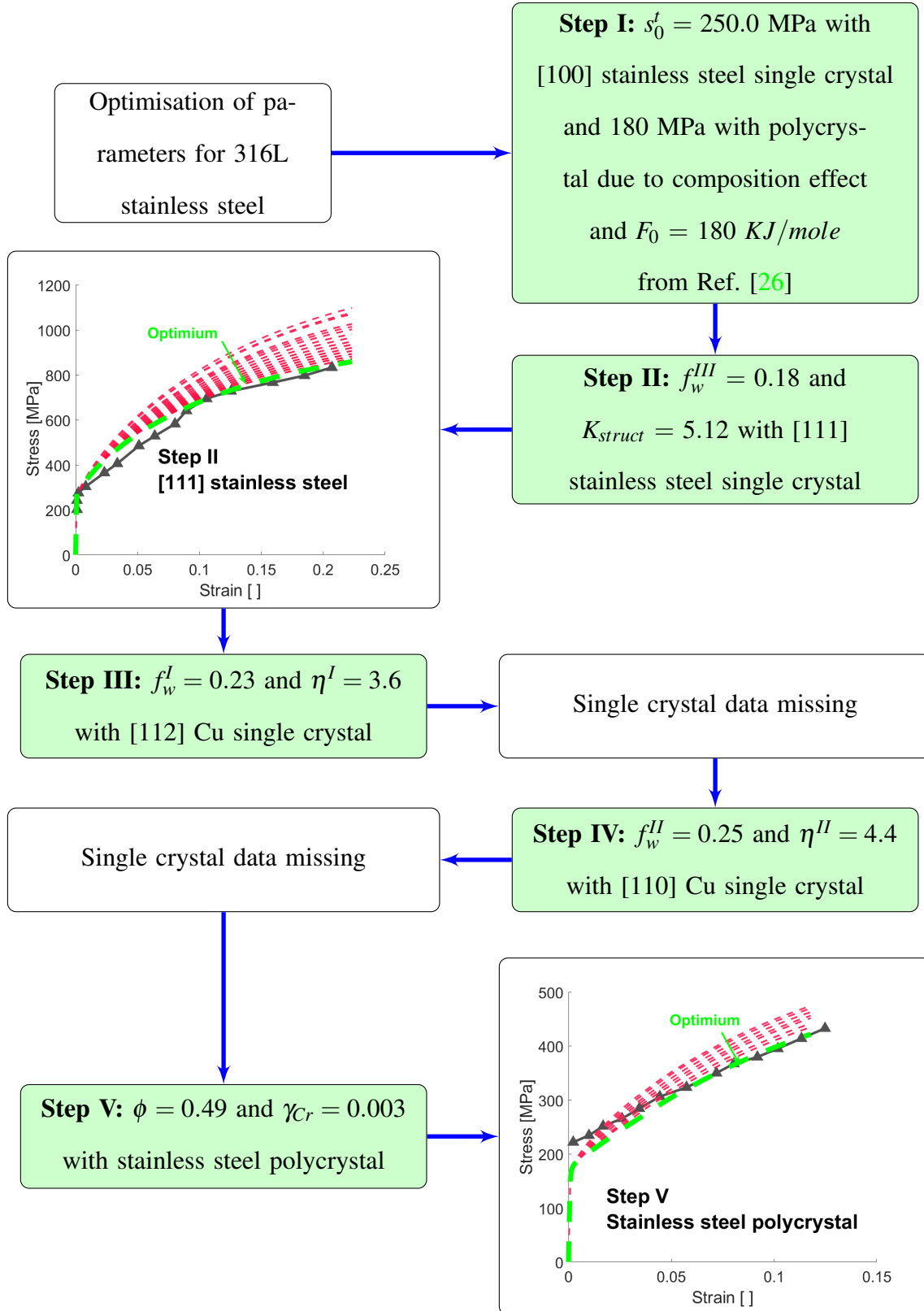


Figure 5.12: Sequential physics-based parameter optimisation for 316L stainless steel. Green lines are predictions with optimised parameters. Red curves are predictions with not-optimised parameters and show the optimisation path. Gray points Experimental data taken from Ref. [27, 28].

Table 5.2: Optimised parameters by new method for Cu, Al, Ni and stainless steel. The optimisation applied for each material independently. s_0^t is in *MPa* and F_0 in *KJ/mole*

Parameters	s_0^t	K_{struct}	f_w^{III}	f_w^I	η^I	f_w^{II}	η^{II}	ϕ	γ_{cr}	F_0
Cu	10	3.94	0.199	0.23	3.6	0.25	4.4	0.48	0.003	150.0
Al	10	4.9	0.19	0.25	2.8	0.25	5.0	0.49	0.003	80.0
Ni	20	4.05	0.19	0.23	4.0	0.25	5.0	0.49	0.001	150.0
Stainless steel	250	5.12	0.18	0.23	3.6	0.25	4.4	0.49	0.003	180.0

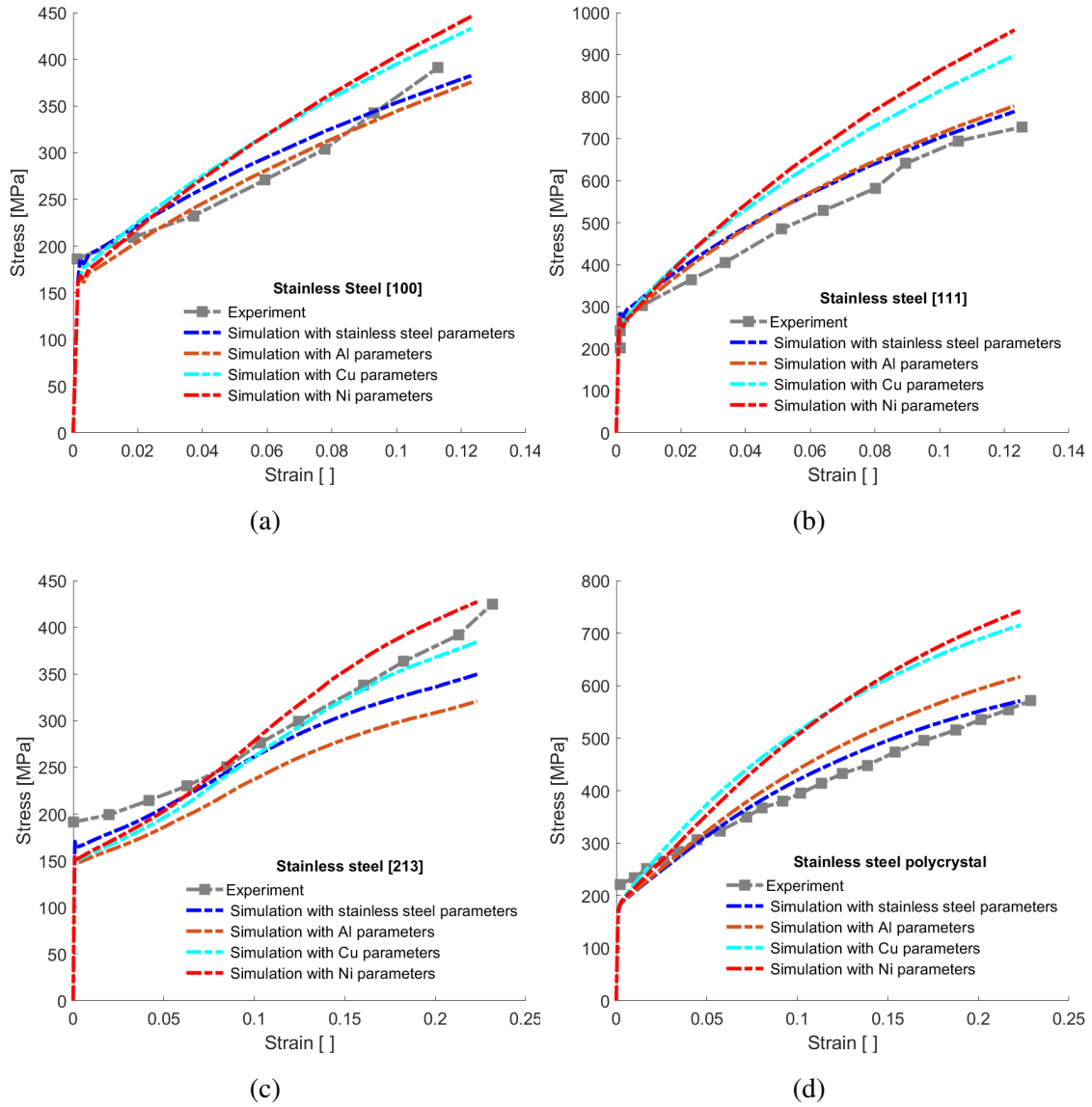


Figure 5.13: Prediction of stress strain curves for stainless steel (316) at 293 K from applying proposed optimization method. Optimised parameters with other FCC materials data, i.e. Cu, Ni and Al can still predict behaviour which shows that mesoscale parameters are material invariant. Experiments from Ref [27,28].

We now use the combined data from Cu, Ni, and Al to apply the suggested optimization strategy. (Figure 5.14). The multi-material simultaneously optimized parameters and predictions are shown in Table 5.3 and Figure 5.15, respectively. Compared to stainless steel parameters predictability, excellent blind predictions with multi-material parameters, represents the applicability of the proposed optimization method for new materials.

In this work, we limited the uncertainty of the optimised parameters by not only fit-

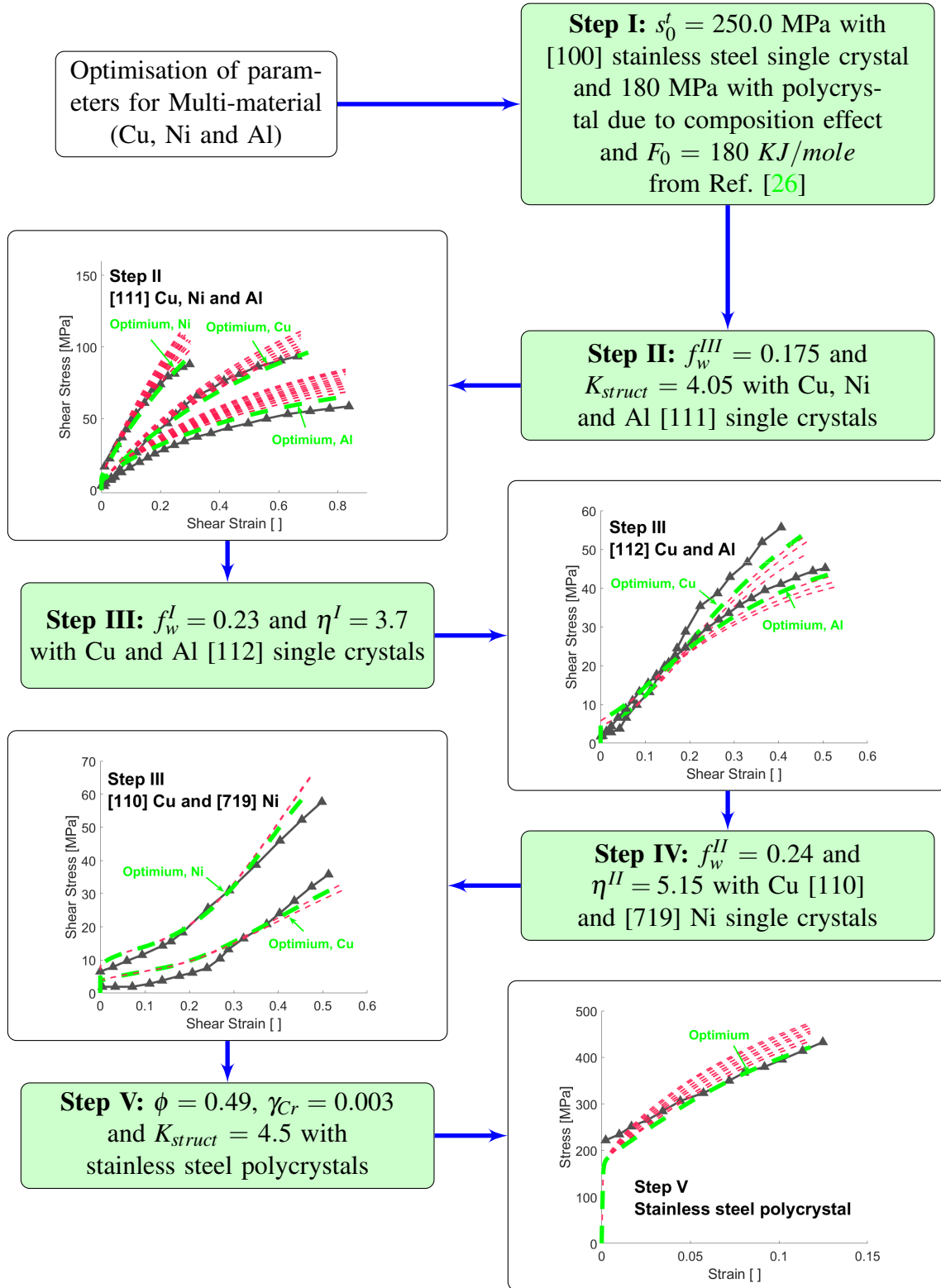


Figure 5.14: Sequential physics-based parameter optimisation for Multi-material (Cu, Ni and Al). Green lines are predictions with optimised parameters. Red curves are predictions with not-optimised parameters and show the optimisation path. Gray points experimental data taken from Ref. [13, 19–22].

Table 5.3: Parameters optimised by proposed method by combining materials data from Cu, Ni and Al simultaneously

Parameters	K_{struct}	f_w^{III}	f_w^I	η^I	f_w^{II}	η^{II}	ϕ	γ_{cr}
By Cu, Ni and Al data	4.5	0.175	0.23	3.7	0.24	5.15	0.49	0.003

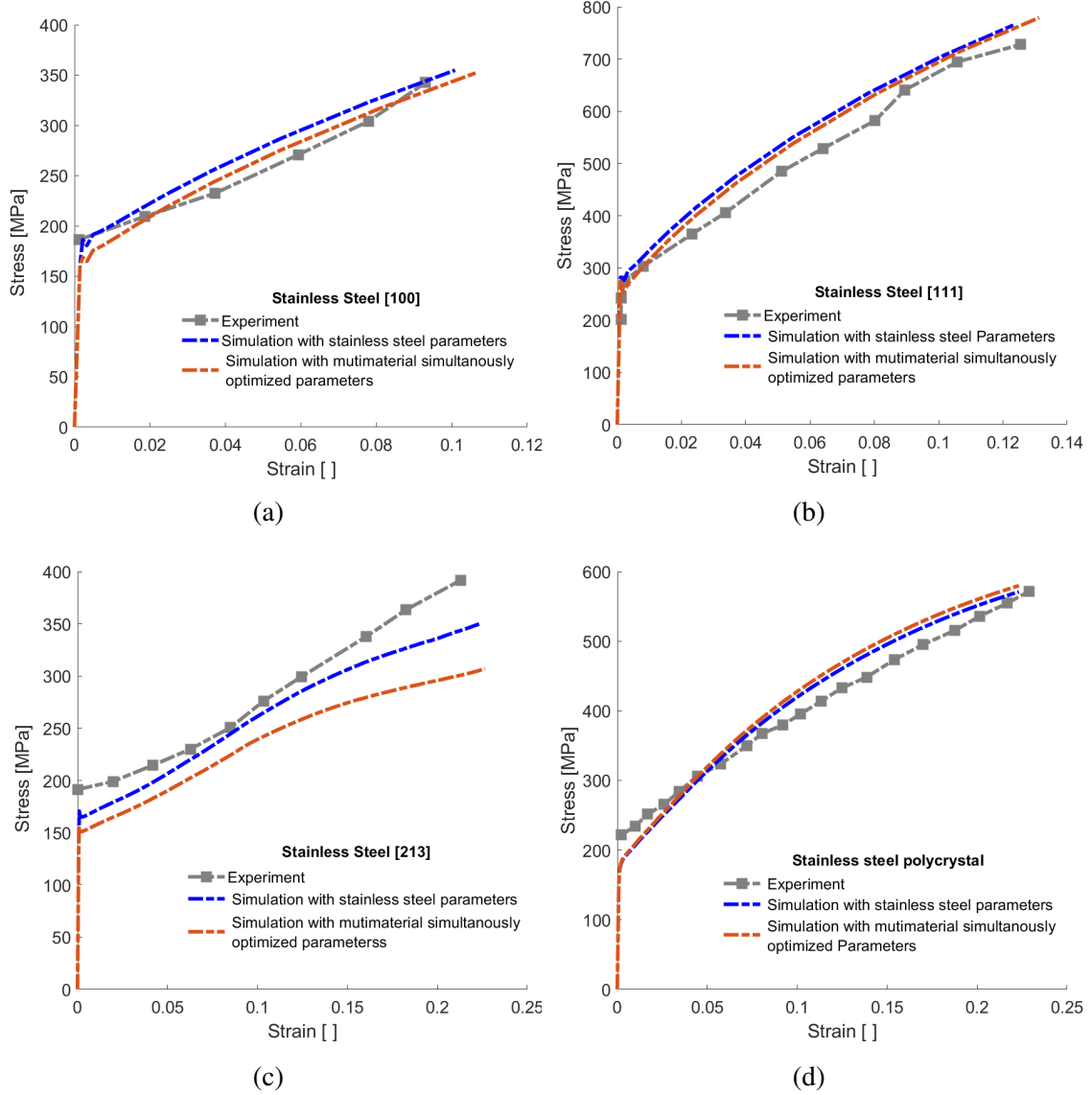


Figure 5.15: Prediction of stress strain curves of stainless steel (316) at 293 K with multi-material (Cu, Ni and Al) simultaneously optimized and stainless steel parameters by the proposed method. Compared to stainless steel parameters predictability, excellent blind predictions with multi-material parameters, represents applicability of the proposed optimization method for new materials with guaranteed predictability. Experiments from Ref [27,28].

ting with macroscopic curves but also independently with mesoscale structures. First, the initial range of parameters was limited by comparison with TEM images before optimisation. Then, we obtained only one set of parameters by capturing both mesoscale structures and macroscale stress-strain curves simultaneously. Usually, the initial range in parameter optimisation is defined by experimental measurements and has a considerable effect on optimised parameter uncertainty. The potential error of the measurements increases parameter uncertainty. In this work, mesoscale parameters are cell aspect ratio, cell wall fraction, and cell size (similitude) which are clear in TEM images and their measurement error is small (Figures 4.4, 4.5, 4.6). In addition to the prediction of stainless steel (Figure 5.15), the upcoming figures represent the predictions of four other materials' single and polycrystal behaviour with only one set of optimised parameters (Table 5.3). Figure 5.16 shows predictions of 14 Cu single crystals behaviour without changing model parameters. Capturing various hardening stages in differently orientated single crystals accompanied with the prediction of the mesoscale structures (Figure 4.11) presents low uncertainty of parameters.

Experimental data requirement for optimisation of model parameters limits crystal plasticity models application. The application for costly, rare, and new materials is not always demanding due to required experiments, particularly for destructive tests. Experiments showed that the mesoscale structures are common in FCC metals, that makes the mesoscale parameters independent of materials [10–12, 15–18, 41]. No need for experiments to obtain material-independent parameters, expands the application of crystal plasticity by the proposed optimisation strategy. We used the unique set of model parameters in Table 5.3 to predict not only stainless steel (Figure 5.15) and Cu (Figure 5.16) but also Ni and Al. Figures 5.17 and 5.18 represent the prediction of Ni and Al single crystal mechanical behaviors (with model parameters in Table 5.3). Agreements with experimental curves describe wide applicability of this optimisation method. We emphasize that only elastic constants, s_0^I , and F_0 were different in these predictions. Elastic constants are measured in the literature and F_0 was obtained by the equation proposed by Ashraf and

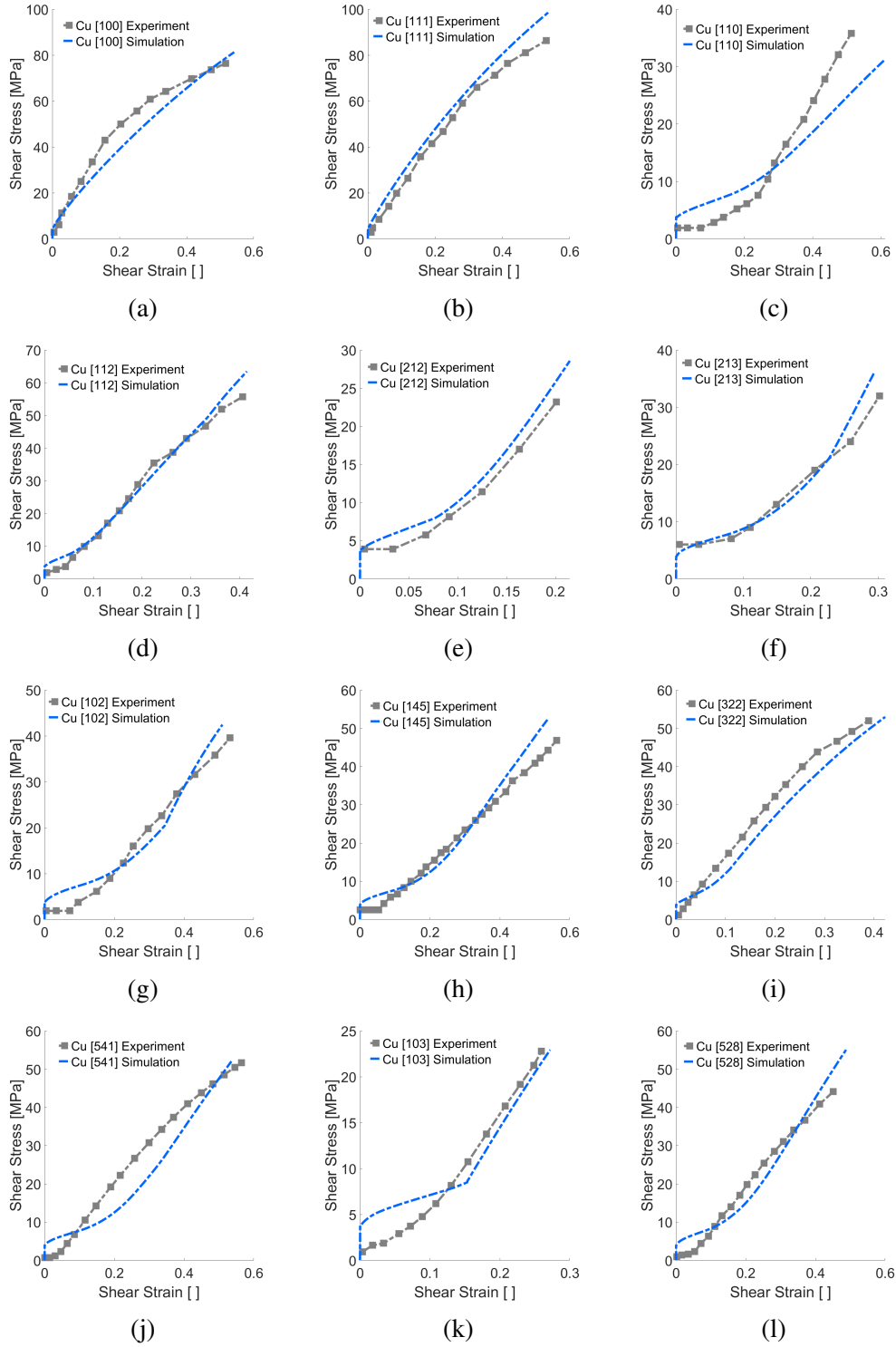


Figure 5.16: Predictions of Cu single crystals behaviour without changing model parameters (optimised parameters listed in Table 5.3). Capturing various hardening stages in differently orientated single crystals accompanied with the prediction of the mesoscale structures (Figure 4.11) presents low uncertainty of parameters. Experiments from Ref [13–15, 29].

Castelluccio [26]. Hence, only parameter s_0^t requires to be optimised for the application of this optimisation method to other FCC materials.

Common optimisation of crystal plasticity parameters by fitting with polycrystal experiments is questionable due to the different behaviors of individual grains (crystals). We discussed this in Chapter 4 and now emphasizing more with predictions of two more materials. Figure 5.15 and 5.19 display the prediction of polycrystalline Cu, Ni, Al, stainless steel, and NiCr20% alloy with the unique set of parameters in Table 5.3. The prediction of polycrystals is based on individual grains' behavior in the proposed optimisation strategy. Therefore, the optimised parameters are predictive for polycrystals with different grain orientations.

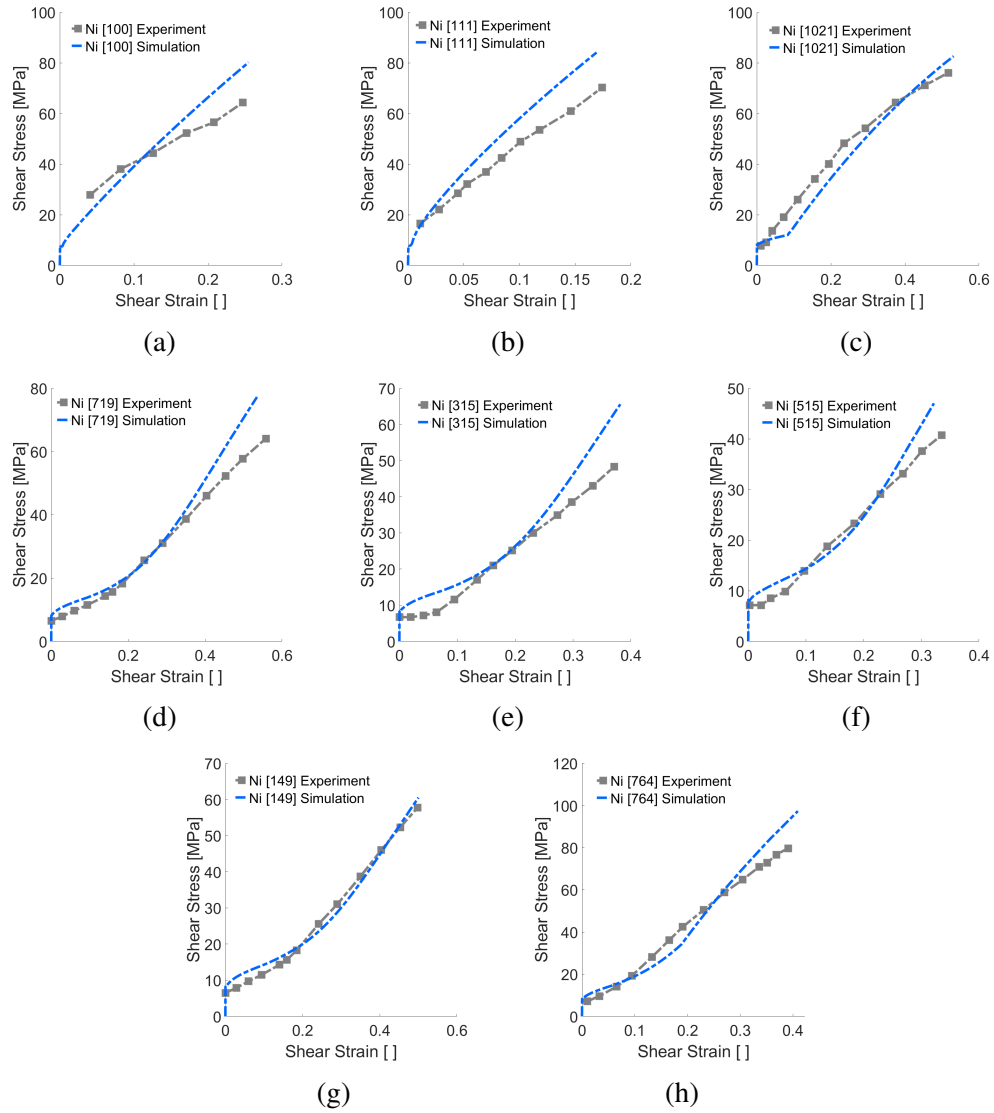


Figure 5.17: Prediction of stress strain curves of Ni single crystals without changing model parameters (optimised parameters listed in Table 5.3). Blind predictions without need for experiment, represents applicability of the proposed optimization method for new materials with guaranteed predictability. Experiments from Ref [19,20].

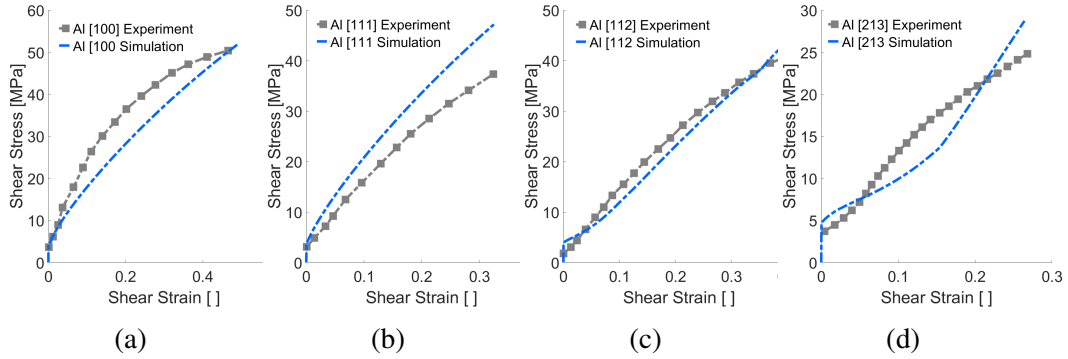


Figure 5.18: Prediction of stress strain curves of Al single crystals without changing model parameters (optimised parameters listed in Table 5.3). Blind predictions without need for experiment, represents applicability of the proposed optimization method for new materials with guaranteed predictability. Experiments from Ref [21, 22].

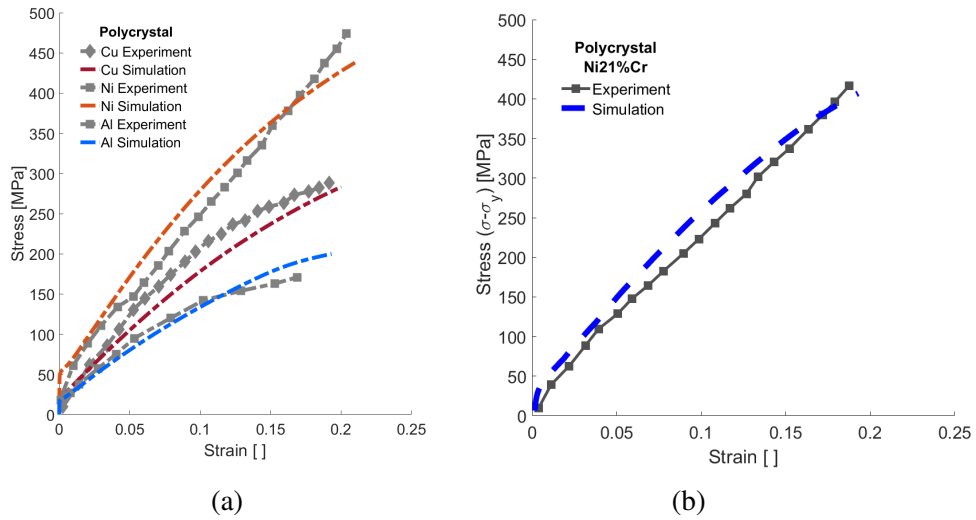


Figure 5.19: Simulation results for polycrystalline Cu, Ni, Al and NiCr with the same unique set of model parameters as single crystals (optimised parameters listed in Table 5.3). The prediction of polycrystals is based on individual grains' behavior in the proposed optimisation strategy. Hence, Optimised parameters are predictive for polycrystals with different grain orientations. Experimental data taken from Ref. [23–25, 30].

5.6 Conclusions

We introduced a new sequential physics-based crystal plasticity parameter optimisation method in this chapter. Optimisation with minimum available experimental data, single objective function, and excellent fitting quality are the advantages of this method.

Furthermore, parameter uncertainty is limited in this method by not only the prediction of macroscopic stress-strain curves but also independently by capturing mesoscale structures. Optimised parameters by this method are material independent which enables the application of this method for new materials without the need for experimental tests for parameter calibration. We used experimental data for Cu, Ni, and Al in this optimisation method to predict the behavior of stainless steel. Results showed that parameters optimised by other FCC materials experimental data are predictive for new materials (stainless steel in this chapter).

Contrary to the common optimisation methods with polycrystal fitting, individual grains/crystals behavior is considered in this strategy. Hence, the optimised parameters are predictive for polycrystals with different grain orientations. Macro- and meso-scale predictions of 29 differently-oriented single- and 5 poly-crystals for 5 materials with only one unique set of model parameters represent the new optimisation method applicability.

Chapter 6

Modeling of Overloads in Cyclic Loading

6.1 Introduction

Fatigue failure has been reported as a main reason for industrial components failure [4]. Fatigue failure occurs by low cyclic loads which are not necessarily uniform and can include monotonic loads between cycles, named overload. Overloads have been shown [30, 32–34, 52, 53] to have a significant effects on micro-scale dislocation substructures as well as macroscopic cyclic deformation. Mariner et al. [30, 34] showed that at fixed applied strain, the saturation cyclic stress amplitude is increased more than 100 percent by application of only 5 percent overload strain in copper, stainless steel 316 and NiCr alloys. They also reported a considerable change in dislocation substructures after overload. Experimental work assessing overloads effect [32–34, 52, 53] are not predictive for other loading conditions and other materials. Hence, a comprehensive analysis requires a mechanistic modelling framework to be able to predict the effect of overloads on subsequent cyclic deformation. The overload models in the literature [54–60] mostly focus on predicting crack growth rate (crack initiation is missing).

Dislocation substructure based models (mesoscale models) were developed for monotonic loading in chapter 4 and for cyclic loading by Castelluccio and McDowell [66]. This chapter applies crystal plasticity by integrating cyclic and monotonic mesoscale models to predict effects of overload on cyclic deformation. Macroscopic stress strain response is controlled mainly by mesoscale substructures in the integrated model. Parameters optimised in Chapter 5 by a novel optimisation method were used to predict Cu single and polycrystals overload response as well as NiCr alloy. Predicted macroscopic responses were explained by mesoscale substructure changes during overload and good agreements were achieved compared with the experiments for both macro and meso scale results. Finally, application of the model to explain the influence of the overloads on fatigue life is discussed.

6.2 Cyclic and Monotonic Models Integration to Predict Overloads Response

An overload in the first cycle (pre-strain or pre-load in the literature [30, 34, 52]) is a monotonic load without history effect by the substructures described in Chapter 4. For overloads with pre-cyclic deformation, we argue that shape of cells which is stable at larger strain amplitudes in cyclic loading, remains unchanged in the overload. However, Chapter 4 showed that transformation of other structures to equiaxed and elongated cells (Type I, II and III structures) is controlled by γ_{Cross} , $\gamma_{Cottrell}$ and γ_{Hirth} in monotonic loading (overload). Veins, PSBs and Labyrinthic can change to Type I, II or III structures in overloads with well developed structures and remain unchanged in overloads by metastable structures. In other words, only well established structures in the overload, i.e. $\eta = \eta^I, \eta^{II}, \eta^{III}$, remain stable at subsequent cycles, otherwise, overload has no effect. Figure 6.1 summarizes changes of cyclic substructures in an overload. The shape change of the substructures affects also the walls spacing, d_{struct} .

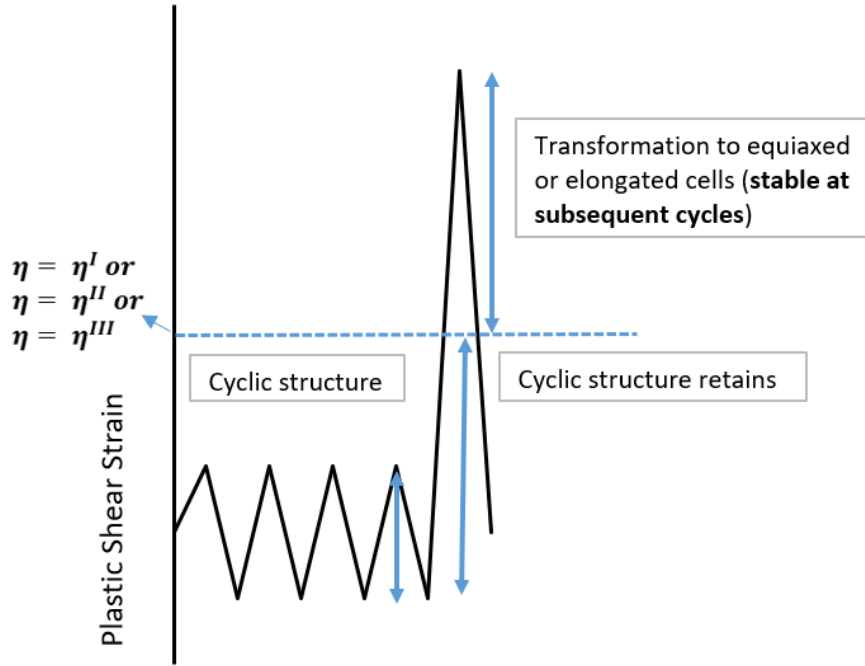


Figure 6.1: Veins, PSBs and Labyrinthic can change to Type I, II or III structures in overloads with well developed structures and remain unchanged in overloads by metastable structures. In other words, only well established structures in the overload, i.e. $\eta = \eta^I, \eta^{II}, \eta^{III}$, remain stable at subsequent cycles, otherwise, overload has no effect.

Activation of slip systems in larger stresses during overloads results in formation of new walls and reduction of mean spacing of sessile dislocations walls, d_{struct} . Figure 6.2 schematically represents that d_{struct} reduces or remains constant depending on either latter slip systems have been activated in pre-cyclic deformation or in the overload. This strategy of changing d_{struct} during overloads is supported by TEM images reported by Li et. al. [31, 32].

Walls are formed in numerous pre-cycles and removing of them in one overload cycle is not physically likely. Hence, increase of wall fraction by adding of new walls is possible ($f_w = \text{Max}(f_w^{Mo}, f_w^{Cy})$). Details of cyclic, monotonic and integrated mesoscale model to predict overload response are shown in Figure 6.3. Prediction of cyclic behavior was based on the cyclic mesoscale model proposed by Castelluccio and McDowell [66]. They used shear strain ranges in slip systems to predict the predominant saturated substructures during cyclic deformation. Similitude equation was used to compute walls spacing and

the walls fraction is computed as,

$$f_w^{Cy} = f_{inf} + (f_0 - f_{inf}) \exp\left(\frac{-\Delta\gamma^{max}}{2g_p}\right) \quad (6.1)$$

where g_p is a model parameter and f_0 and f_{inf} are initial and saturated walls fractions, respectively (Figure 6.3).

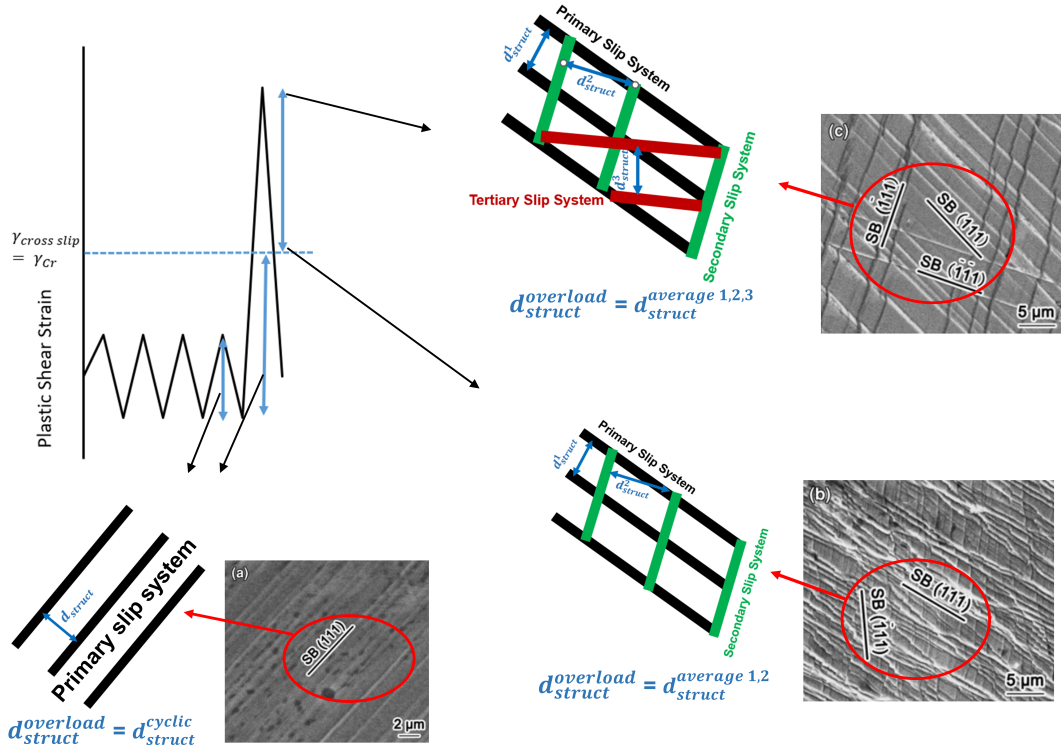


Figure 6.2: Evolution of walls spacing, d_{struct} , during overloads. d_{struct} reduces or remains constant depending on either latter slip systems (secondary, tertiary, etc.) have been activated in pre-cyclic deformation or in the overload. We believe that activation of new slip systems in larger stresses during overloads results in formation of new walls (green and red lines) and reduction of d_{struct} . This strategy of changing d_{struct} during overloads are satisfied by TEM images reported by Li et. al. [31, 32]. The TEM images from Ref. [31].

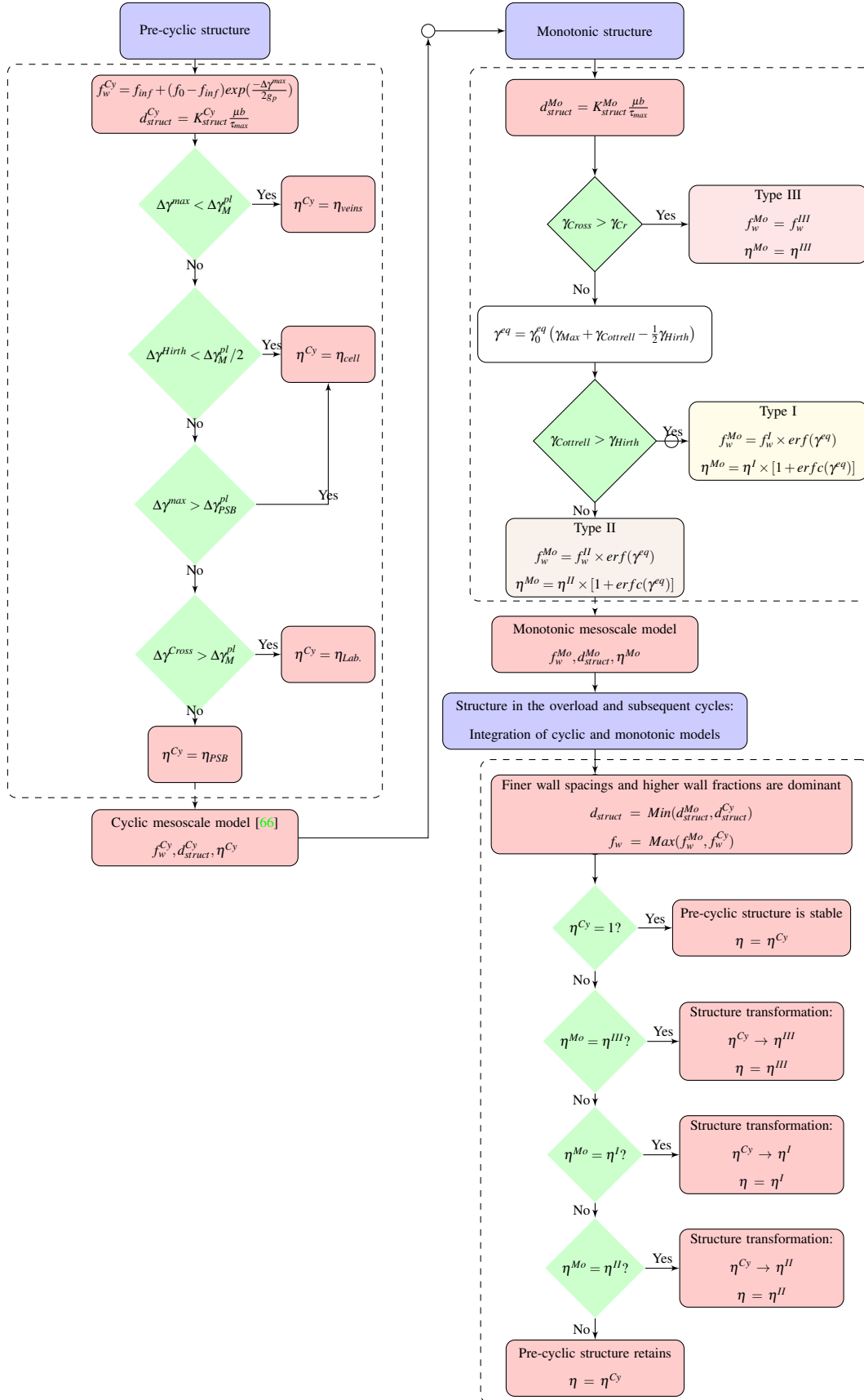


Figure 6.3: Effect of overloads on dislocation substructures in cyclic loading: integration of cyclic and monotonic models.

Proposed substructures during overloads (Figure 6.3) are confirmed also by substructural analysis in experimental TEM images. Figure 6.4 shows the evolution of various cyclic substructures during overloads from experiments. As can be seen, Veins, PSBs and Labyrinthic substructures are retained up to five percent and transformed to equiaxed and elongated cells at ten percent overload.

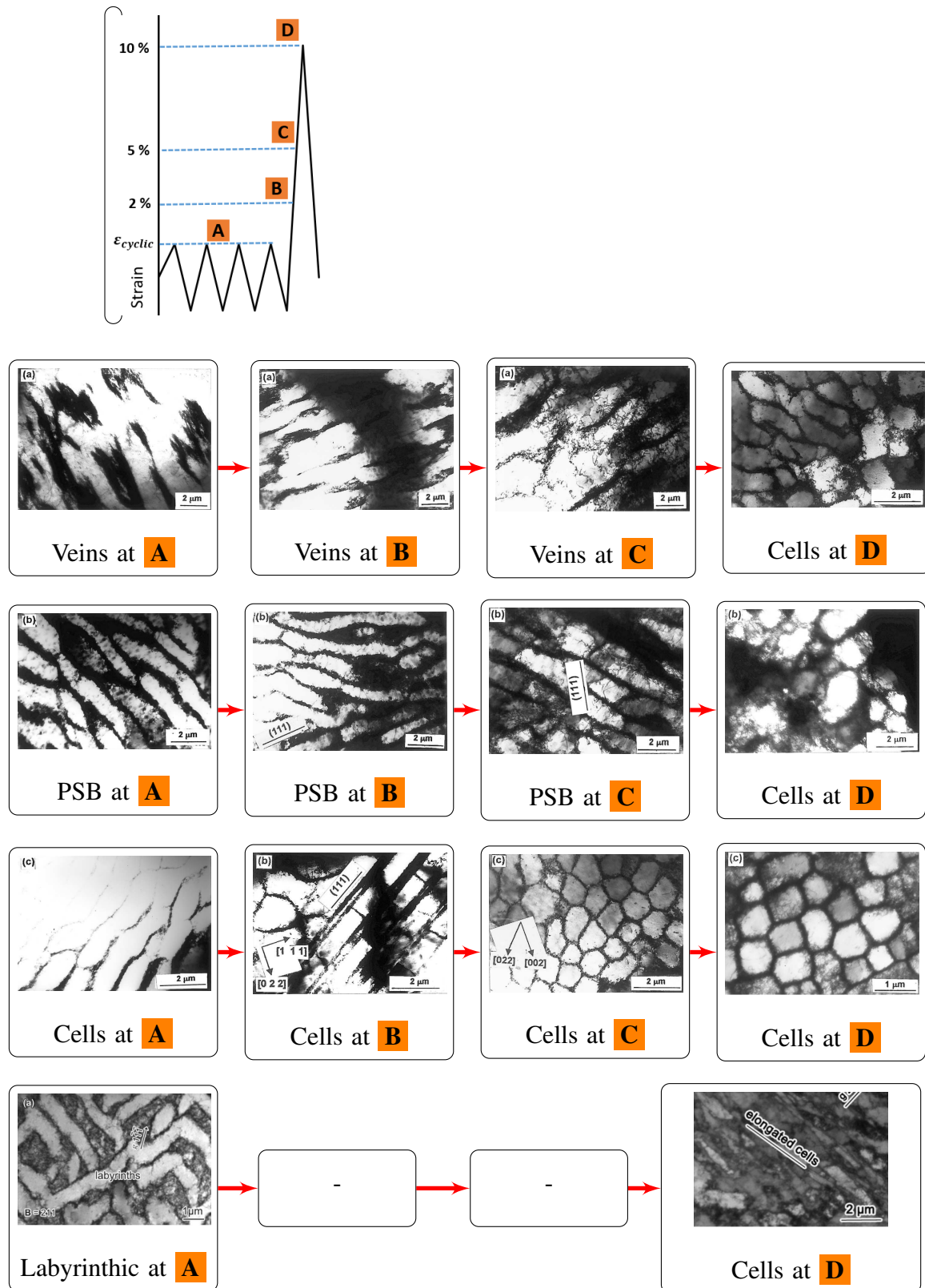


Figure 6.4: Evolution of various cyclic substructures during overloads. Veins, PSBs and Labyrinthic substructures are retained up to five percent and transformed to equiaxed and elongated cells at ten percent overload. The TEM images from Ref. [31,33].

6.3 The Model Parameters and Implementation

Cyclic mesoscale parameters are listed in Table 6.1 (all other parameters follow those in Chapter 4). Since numerous cycles (>200) are needed to saturate substructures in experimental cyclic loading, we added an acceleration factor (10-200) to dislocation density evolution in Equation (3.22) to accelerate the structure saturation. We argue that for experimental structures saturates in 200 cycles the acceleration factor of 10 is needed for the simulations to saturate the structures in 20 simulation cycles ($200 = 10 \times 20$).

Table 6.1: Cyclic mesoscale model parameters.

Parameter	Values
Similitude coefficient, K_{struct}	2.75
Platue plastic shear range, ΔG_M^{pl}	$1 \times 10^{-5} - 7 \times 10^{-4}$
PSBs upperbound shear, ΔG_{PSB}^{pl}	0.018
The wall fraction change rate parameter, g_P	0.002
The initial wall fraction, f_0	0.45
The final wall fraction, f_{inf}	0.15
Veins aspect ratio, η_{Veins}	50.0
PSBs aspect ratio, η_{PSBs}	15.0
Cells aspect ratio, η_{Cells}	1.0
Labyrinthic aspect ratio, $\eta_{Lab.}$	5.0

6.4 Results and Discussion

6.4.1 Application to Cu

First, we apply the model to predict the response of Cu during overloads. Figure 6.5 represents the prediction of overload response for [017] Cu single slip crystal. The predicted stress-strain curves of unfatigued tension and overloads after 7×10^{-4} and 3×10^{-3} pre-cyclic strain amplitudes are shown in Figure 6.5a. Hardening Stage I is evident in unfatigued curve of Figure 6.5a (blue curve). However, as mentioned in Ref. [31], Stage I is

missing in experimental curve of Figure 6.5d.

The predicted and experimental [31] substructures in 7×10^{-4} and 3×10^{-3} cyclic strain amplitudes are Labyrinthic and cells, respectively. While the Labyrinthic structure provides long enough dislocation mean free path ($\eta_{Lab.} = 5.0$) to see Stage I in the next overload (black curves in Figure 6.5), Stage I disappears by cells formed in prior cycles (orange curves in Figure 6.5). Not only the hardening stages, but also yield stress is affected by substructures developed in pre-cyclic deformation. Jia and Fernandes [33] showed that finer structures of pre-cyclic deformation increase the yield stress in the next overload. Increase of the yield stress due to prior finer structures shown in Figure 6.5b explains higher stresses in overload results in Figure 6.5a which is not evident in experiments in Figure 6.5d.

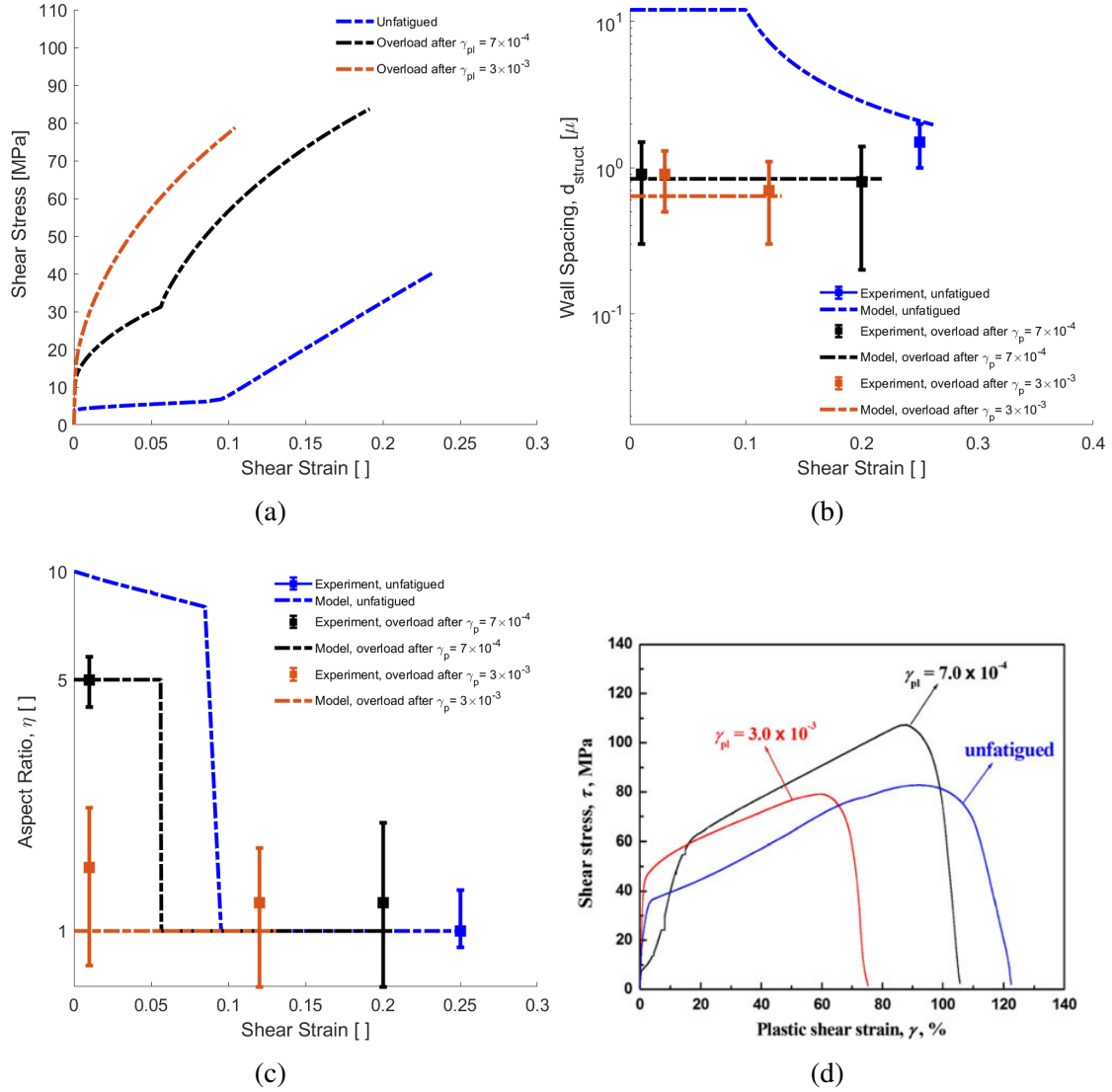


Figure 6.5: Predicted overload response at multi-scales for [017] Cu single slip crystal. a) Predicted stress-strain curves of unfatigued tension and overloads after 7×10^{-4} and 3×10^{-3} pre-cyclic strain amplitudes. b) Wall spacing, c) Structures aspect ratio and d) Experimental stress strain curves. While Labyrinthic structure provides long enough dislocation mean free path ($\eta_{Lab.} = 5.0$) to see Stage I in the next overload (black curves), Stage I disappears by cells formed in prior cycles (orange curves). Increase of yield stress due to prior finer structures explains higher stresses in model stress strain results which is not evident in experiments. Experiments from Ref. [31].

Prediction of single crystals or grains results in reliable prediction of polycrystals. Results after five and ten percent overloads in Cu polycrystals are represented in Figure 6.6. The predicted and experimental dominant substructures by current model after five and ten percent overloads (Figure 6.6c and 6.6d) are ≈ 2 and $\approx 1 \mu$ cells, respectively.

Compared to five percent overload, finer cell size (wall spacing) in ten percent ($\approx 1\mu$) results in higher stresses. As can be seen, effect of overloads is different at low and high strain amplitudes.

At low strain amplitudes: increase of the stress is due to transformation of Veins and PSBs of virgin material to cells in overloads. **At high strain amplitudes:** cells are dominant structures in virgin material. Hence the overload has no effects from structural shape changes after five and ten percent overloads. However, wall spacing is decreased after ten percent overload to $\approx 1\mu$ (Figure 6.6d) which describes the stress increase. Unchanged structure shape and wall spacing, explain marginal change of the stress after five percent overload.

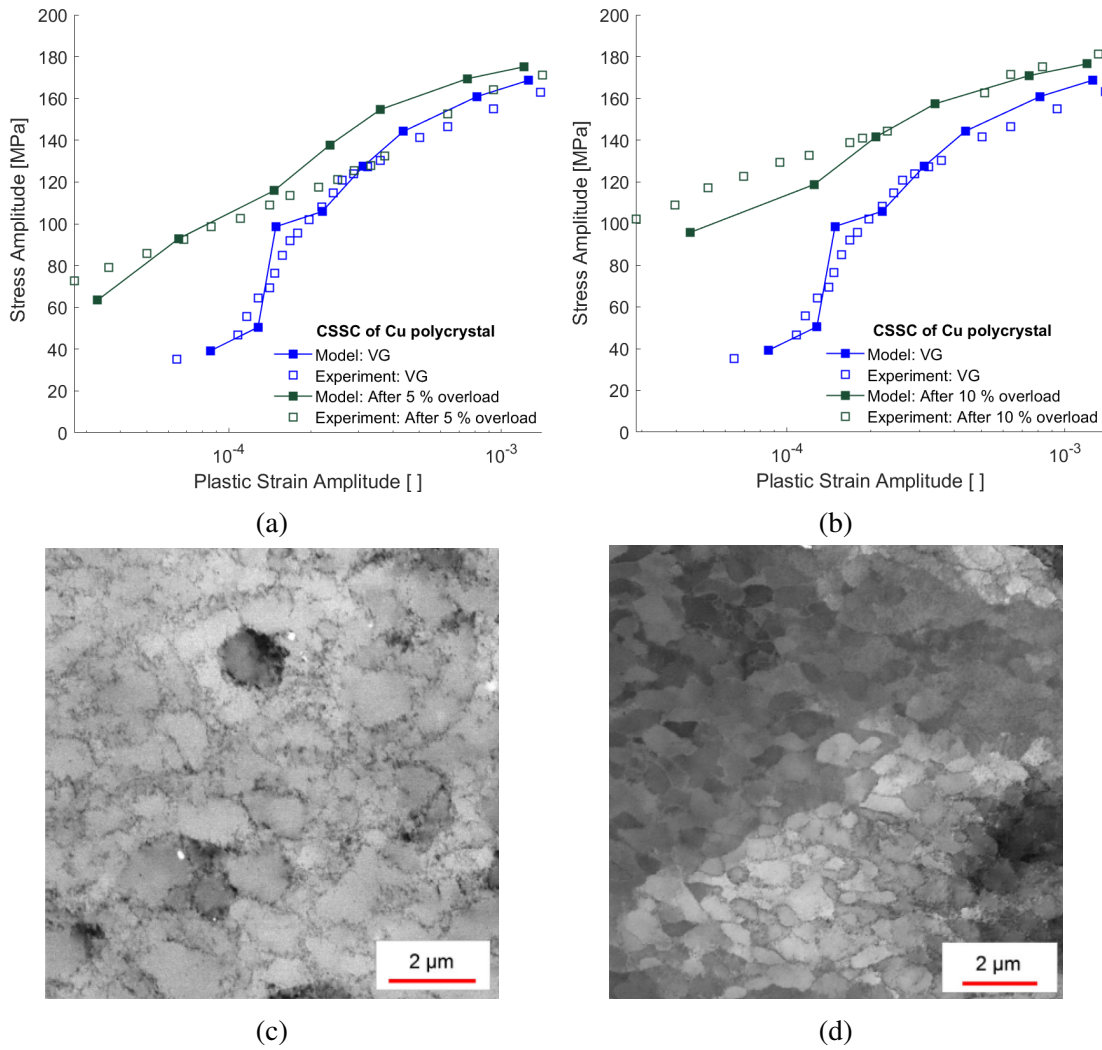


Figure 6.6: CSSCs of virgin (VG) material, after a) Five and b) Ten percent overload of Cu polycrystals. Predicted dominant substructures by current model after c) Five and d) Ten percent overloads are ≈ 2 and $\approx 1\mu$ cells, respectively. Increase of the stress at low strain amplitudes is due to transformation of Veins and PSBs of virgin material to cells in overloads. Compared to five percent overload, finer cell size in ten percent ($\approx 1\mu$) results in higher stresses. Experiments from Ref. [30].

6.4.2 Application to NiCr Alloy by Parameters Optimised by Cu Data

Chapter 5 explains that optimisation of material invariant parameters enables prediction of new materials behaviour by parameters estimated by other FCC materials experimental data. We predicted overload effects on subsequent cyclic deformation for NiCr alloy with model parameters optimised by Cu experimental data (Table 5.1). Chemical composition

of this alloy are listed in Table 6.2. We argue that prediction of monotonic and cyclic responses (Figure 6.7a and 6.7b) is necessary for robust prediction of integrated overload model. Figure 6.7b represents blind prediction (without experimental data for parameters calibration) of overloads effect for 14 percent overload in polycrystalline NiCr alloy. Dominant cell structure after the overload is shown in Figure 6.7c. Transformation of Veins and PSBs to cells in the overload increases the stress at subsequent cycles.

Table 6.2: Chemical composition (wt%) of NiCr alloy modelled in this chapter, [34].

Ni	Cr	Si	Fe	Mn
77.2	20.9	1.4	0.2	0.3

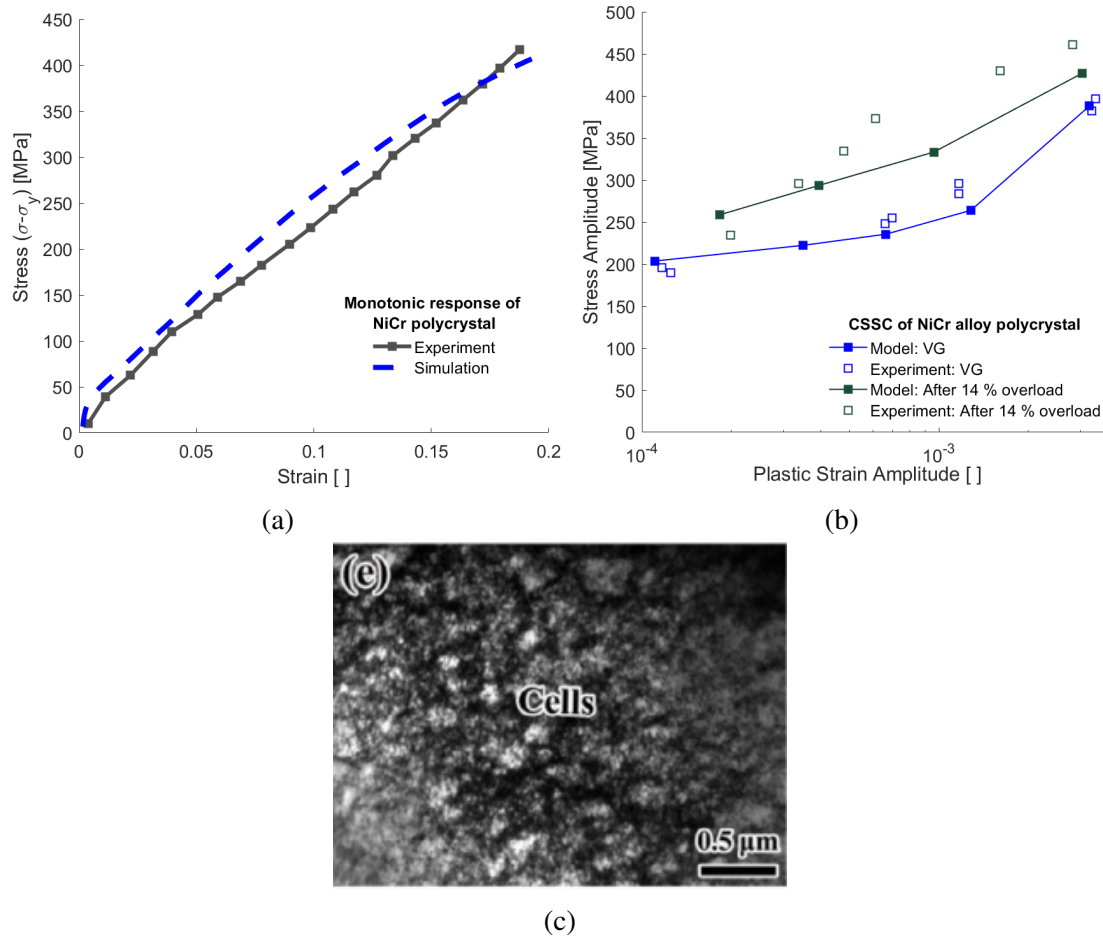


Figure 6.7: a) Prediction of monotonic response of NiCr polycrystal. b) CSSCs of virgin (VG) material and after 14 percent overload of this alloys and and b) Cell structure after the overload. Transformation of Veins and PSBs to cells in the overload increases the stress at subsequent cycles. Experiments from Ref. [34,35].

6.4.3 Crystal/Grain Orientation Effect

Applied overloads strain range and loading direction are key factors that define overload effects on subsequent cyclic deformation. Here, we analyse the effect of applied strain and crystal/grain orientations on overloads response. Figure 6.8 shows the effects of overloads on cyclic deformation for various Cu single crystals. While five percent overload is not sufficient to change the structure in [112] crystal, PSBs formed in pre-cycles transformed to elongated cells (Type I) in ten percent overload, Figure 6.8a. In [110] crystal with longer hardening Stage I, Figure 4.10, higher overloads are needed to evolve the struc-

ture. Accordingly, PSBs are stable even after 20 percent, but altered to elongated cells (Type II) in 30 percent overload, Figure 6.8b. Labyrinthic structure in [100] crystal is changed to equiaxed cells even in five percent overload, Figure 6.8c. However, since the change of structures aspect ratio in [112] and [110] single slip crystals is higher than the change in [100] crystal ($\eta^{PSB} \rightarrow \eta^{I,II} > \eta^{Lab} \rightarrow \eta^{III}$), the increase of the stress due to overload is larger. Cell structure in [111] multiple slip crystal is stable even in 30 percent overload and stress remained unchanged, Figure 6.8d. These results supports that the effect of overloads will be marginal for textured polycrystals with more grains near [111] and [100] orientations and noticeable for those with more single slip grains. Structure transformation in the overload not only changes the stress but also affects subsequent fatigue life.

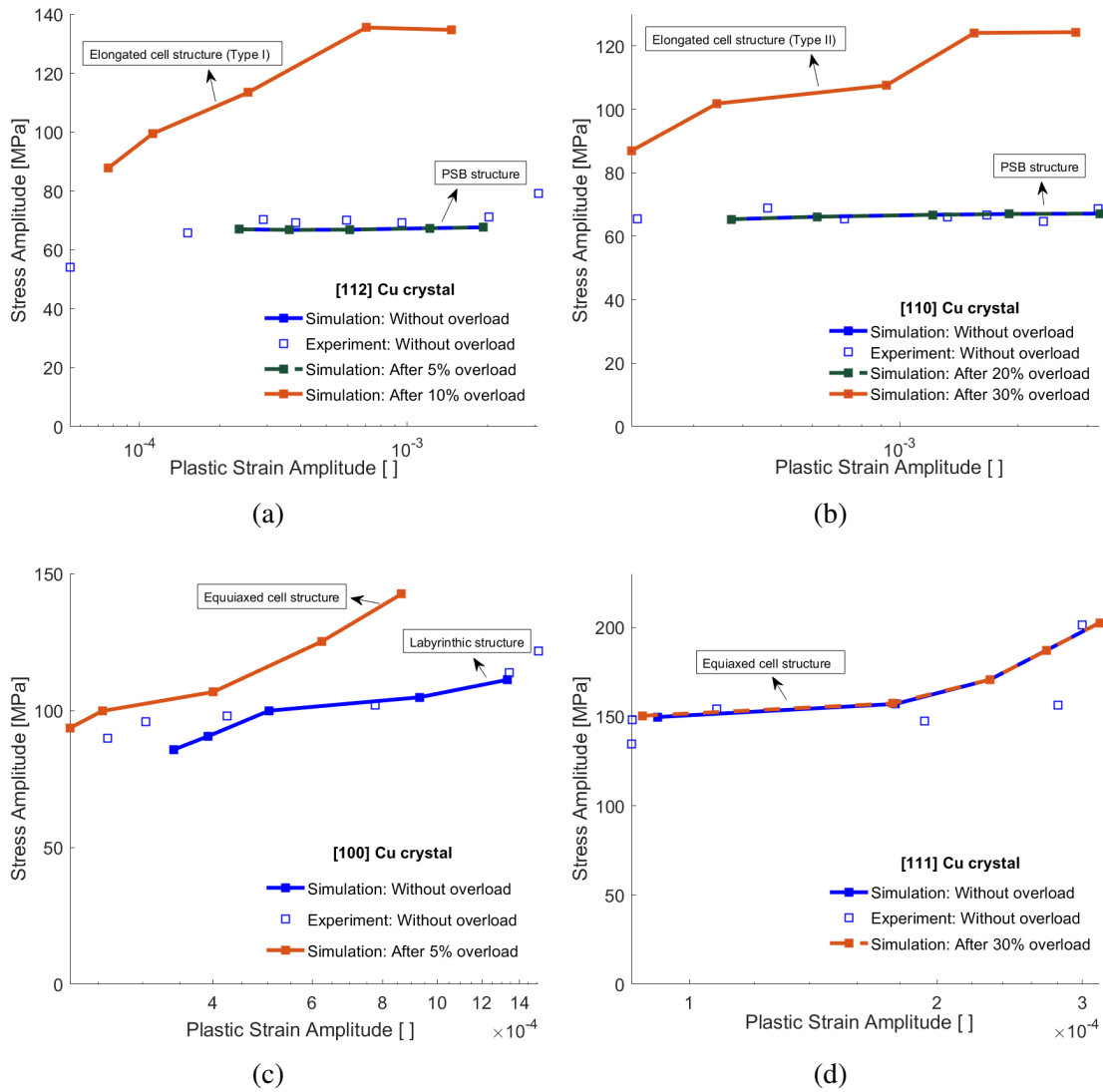


Figure 6.8: Predicted effects of overloads on cyclic deformation for a) [112] b) [110] c) [100] and [111] Cu single crystals. While five percent overload is not sufficient to change the structure in [112] crystal, PSBs formed in pre-cycles transformed to elongated cells (Type I) in ten percent overload. In [110] crystal with longer hardening Stage I, Figure 4.10, higher overloads are needed to evolve the structure. Accordingly, PSBs are stable even after 20 percent, but altered to elongated cells (Type II) in 30 percent overload. Labyrinthine structure in [100] crystal is changed to equiaxed cells even in five percent overload. Cell structure in [111] multiple slip crystal is stable even in 30 percent overload and stress remained unchanged. Experiments from Ref. [36–39].

FIP parameters have been proposed in the literature for microstructural fatigue crack initiation and growth, [118, 119]. A direct relation with shear strain range is common in most definitions (e.g., $FIP \propto \Delta\gamma$). At constant applied stress, transformation of long structures (Veins, PSBs and Lab.) to cells during overloads, decreases the shear strain

range and FIP at subsequent cycles which results in longer fatigue life. Accordingly, overloads can have noticeable improvement effects on subsequent fatigue life of textured polycrystals with more grains near single slip directions . Fatigue life improvements after overloads have been also reported by several experimental and modelling works [59, 120–124]. Further work needs to be done for accurate prediction of the effect of overloads on subsequent fatigue life.

6.5 Conclusion

This chapter integrated cyclic and monotonic mesoscale models to predict the effect of overloads on subsequent cyclic deformation. It was shown that the structure transformation during overloads predicts macroscopic response. The proposed model was applied to Cu single and poly-crystals and NiCr alloy polycrystals. Macro and meso-scales results were in agreement with experiments. Macroscopic response is explained based on substructures shape, wall spacing and wall fraction. The model was also applied to predict overload response of NiCr alloy by the parameters optimised by Cu experimental data.

The analysis of overloads with different applied strains and in various crystal orientations showed that overloads have improvement effects on subsequent fatigue life. These effects are marginal in multiple slips and noticeable in single slip crystals due to structure transformation. The proposed substructure based model is a robust tool for blind prediction of overload response for new materials without single crystal experimental data.

Chapter 7

Discussions and Implications of the Overall Work

7.1 Discussions

The cyclic behavior of metals is controlled by mesoscale structures formed over hundreds or thousands of cycles. Cyclic mesoscale structures can change by a monotonic overload, which are common in engineering applications. Hence, we contend that current models that do not incorporate the relationship between macro- and meso-scales are less reliable. This multiscale relationship been modeled by the crystal plasticity framework.

However, the predictability of crystal plasticity models is questionable due to the large number of parameters with unknown uncertainties. We argue that crystal plasticity models just fits the experimental stress-strain curves do not necessarily validate the model and parameters. For example, Figure 7.1a shows the failure of the model to predict Ni [8111] crystal with the parameters in Table 5.3. We changed only one parameter (γ_0^{eq}) and captured the curve (Figure 7.1b). While the value predicts this crystal with excellent fitting quality, it is not predictive for all 29 single- and 5 poly-crystals in Chapter 5. The uncertainty of parameters in this work has been bounded by not only fitting experimental stress-strain curves but also independent prediction of mesoscale structures. Since the model and parameters have been already verified, we looked into any other possible error sources in Figure 7.1a. A comparison of the macroscopic and mesoscale experiments for Ni [8111] and its surrounding crystals in Figure 7.1c and 7.1d shows that the experimental curve for [8111] is probably incorrect.

Potential experimental errors and different material internal states (initial dislocation density and substructure, crystal orientation, chemical composition, etc.) make the experiments different. Figure 7.2 and 7.3 represent experimental stress-strain curves for Cu in monotonic and cyclic loadings, respectively. Experiments present variability even though the reported material and crystal orientations are the same ([100] in Figure 7.2a, [111] in 7.2b, and [100] in 7.2c). When the complexity of polycrystal is additionally introduced, the experimental variabilities are more pronounced (Figure 7.3). Variability in reported experiments demand a multiscale model to consider the experimental errors and material internal states. Therefore, we emphasize that parameter calibration just by

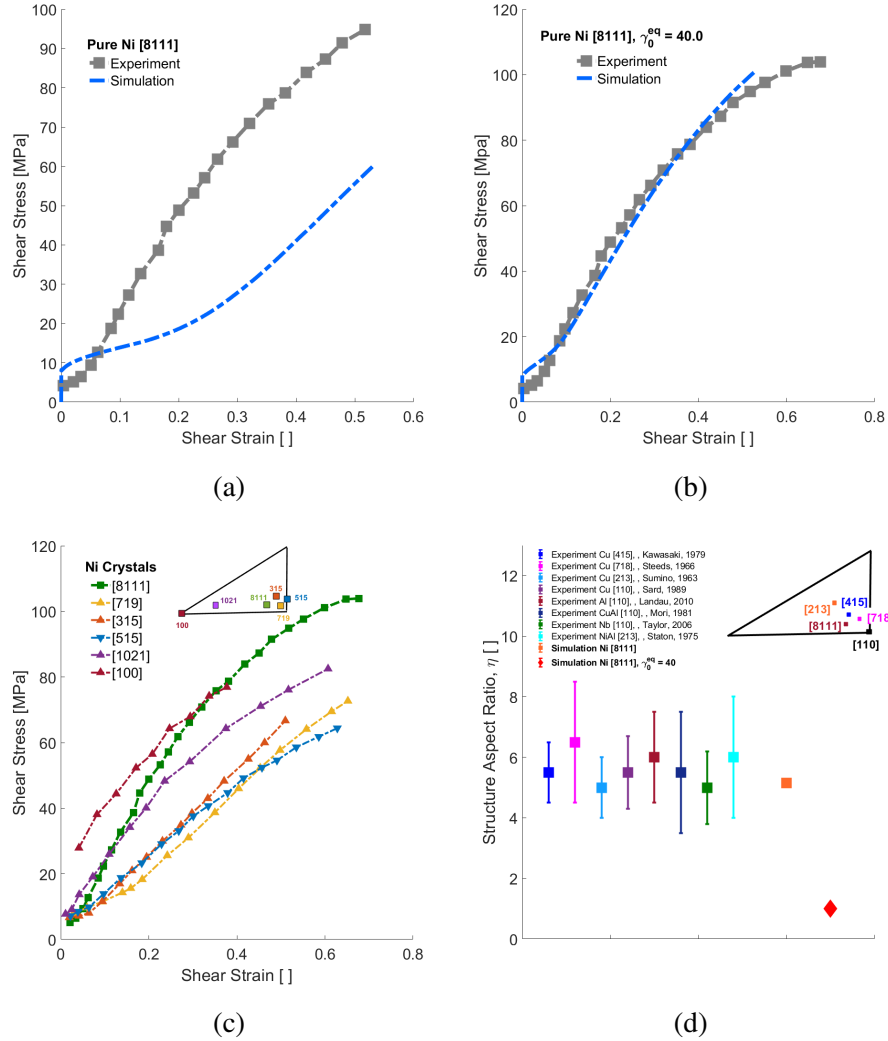


Figure 7.1: a) Fail to predict Ni [8111] crystal, b) Prediction of [8111] crystal with wrong parameters ($\gamma_0^{eq} = 40.0$), c) Experimental stress-strain curves for other Ni crystals in the neighbourhood of [8111] and d) Mesoscale structure of FCC crystals in the neighbourhood of [8111]. Both macroscopic curves and mesoscale structures show that the experimental [8111] curves is incorrect. Experiments from Ref [10, 14, 18–20, 40, 41, 125–128].

fitting with polycrystal curves, without considering individual crystals orientation, is not reliable. Figure 7.4a shows an experimental analysis of the influence of crystal orientation. We repeated the same analysis for more crystals (Figure 7.4b). We argue the typical underestimation of the crystal orientation effect in parameter optimization by only fitting polycrystal curves.

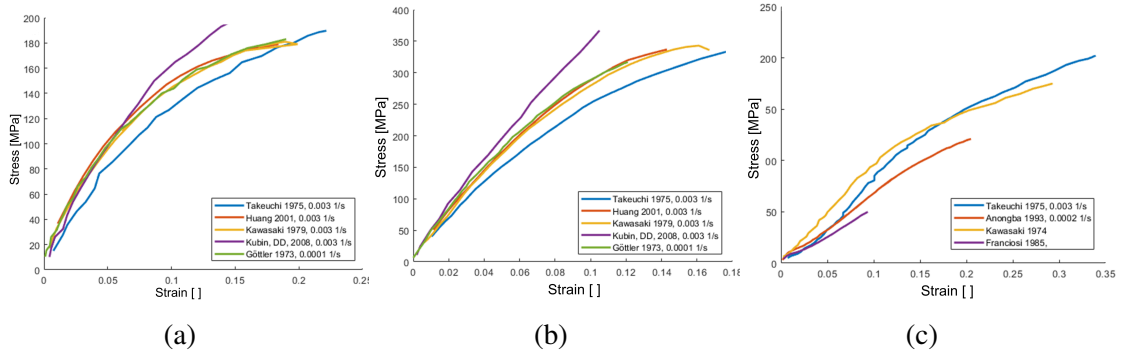


Figure 7.2: Variability in reported experimental results for a) [100], b) [111] and c) [112] Cu single crystals in monotonic loading. Experiments from Ref. [11, 13, 17, 41–44].

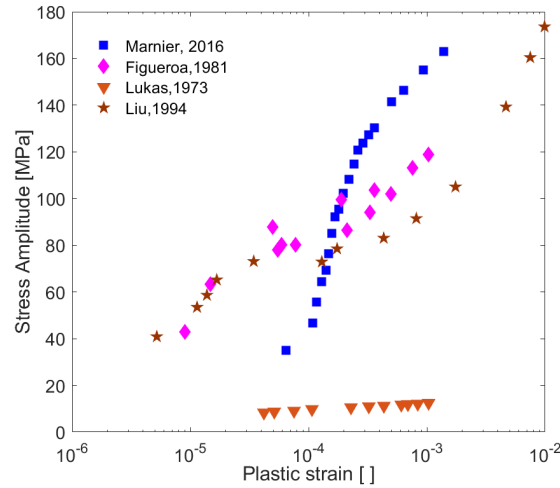


Figure 7.3: Variability in reported experimental results for polycrystalline Cu in cyclic loading. Experiments from Ref. [30, 45–47].

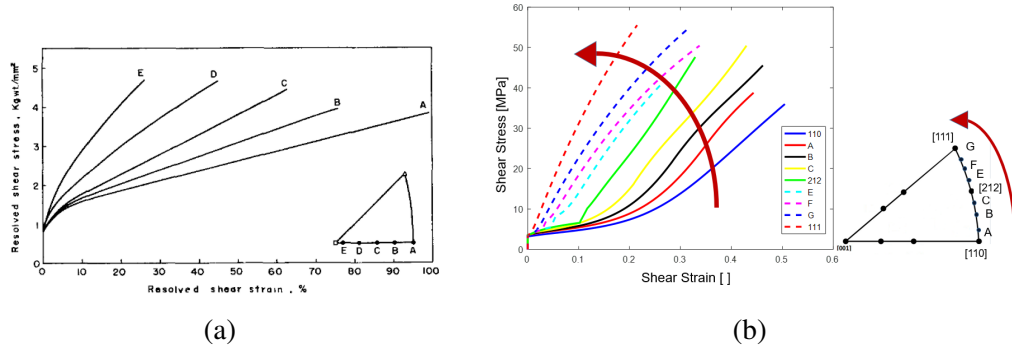


Figure 7.4: Crystal orientation sensitivity analysis by a) Experiment by Sumino and Yamamoto [48] and b) Current model. We argue the typical underestimation of the crystal orientation effect in parameter optimization by only fitting polycrystal curves.

Due to the importance of crystal orientation, any potential errors in measured crystal orientation, complicate model predictions. Therefore, the inaccurate orientation for the Ni [8111] crystal is the probable reason for the failure of the model prediction in Figure 7.1a and also the difference with surrounding crystals in Figure 7.1c and 7.1d. To investigate that, we repeated the simulation for 400 crystals in the 0-5 degree, 400 in the 0-10 degree, and 400 in the 0-20 degree neighborhood of the [8111] crystal. Macroscopic and mesoscale results are shown in Figure 7.5. The stable mesoscale structure for crystals in the vicinity of [8111] is a Type-II structure with $\eta^{II} = 5.15$. This is confirmed by experiments in Figure 7.1d and simulations in Figure 7.5d. In spite of no structure transformation for crystals in 0-5 degree misorientation (Figure 7.5d), the stress variability is more than 70 percent (Figure 7.5a). The stress variability was raised significantly by the structure transformation (Type-II to Type-III and Type-I in Figure 7.5e) in some crystals with 0-10 degree misorientation above 0.17 percent deformation. (Figure 7.5b). Structure transformations from Type-II to Type-I and Type-III, change the structure aspect ratio from $\eta^{II} = 5.15$ to $\eta^I = 3.7$ and $\eta^{III} = 1.0$, respectively. The reduction of the structure aspect ratio raises the stress by increasing mobile dislocation density. Hence, the stress was increased more in crystals with Type-II to Type-III transformation. Figure 7.5f demonstrates that both structure transformations occur earlier (0.05 percent deformation) in crystals with 0-20 degree misorientation. Thus, more than 10-degree misorientation

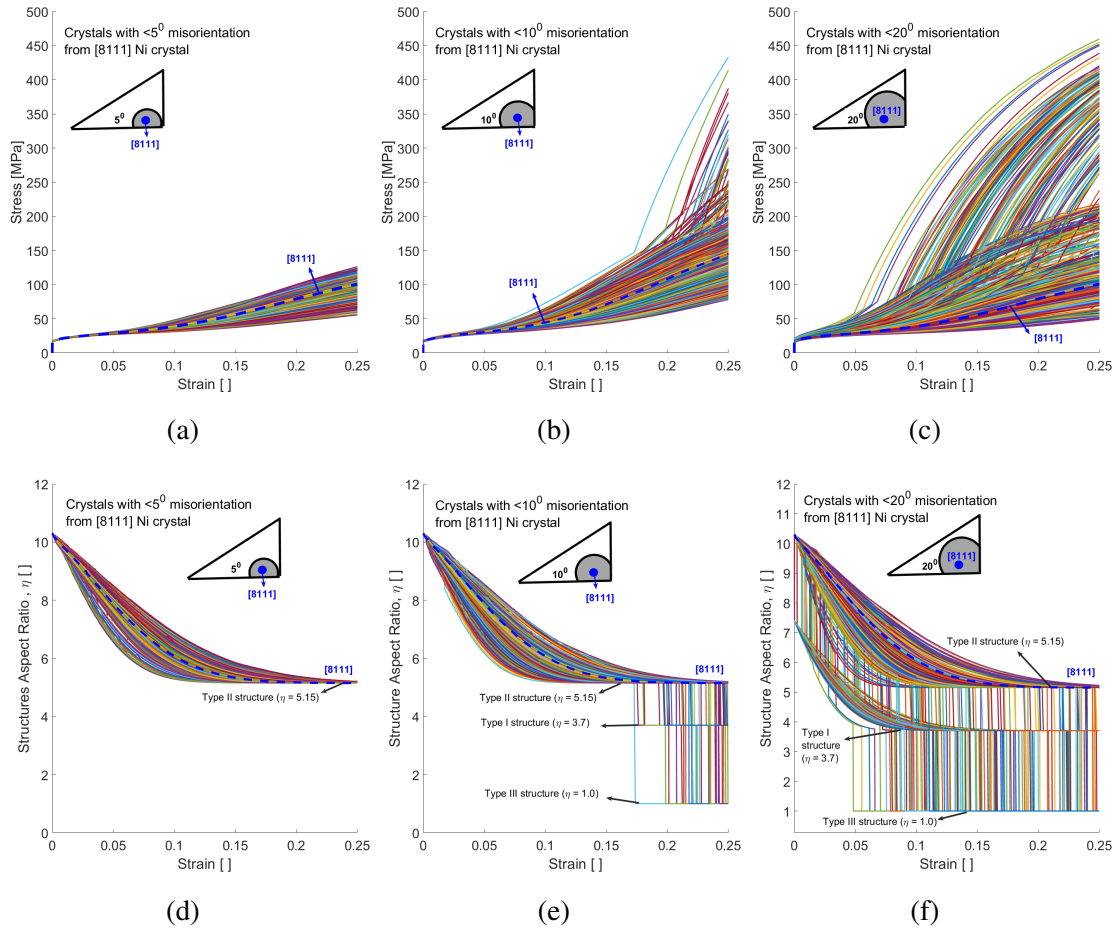


Figure 7.5: Effect of misorientation from [8111] Ni crystal on mesoscale structure (d-f) and macroscopic stress-strain curves (a-c). a and d) 0 – 5°, b and e) 0 – 10° and c and f) 0 – 20° misorientation. More than 10-degree misorientation entirely changes the mesoscale structure and the macroscopic response. As a result, the crystal orientation must be determined and reported in experiments with a high degree of accuracy. Experiment from Ref [40].

entirely changes the mesoscale structure and the macroscopic response (Figure 7.5c). As a result, the crystal orientation must be determined and reported in experiments with a high degree of accuracy.

The predictability of the model was further improved by incorporating the probable orientation error in some experiments. The judgment about the possible experimental error is being done by both macroscopic stress-strain response and mesoscale structure. Figure 7.6 represent the prediction of NiCr alloys single crystals by attributing the error to the crystal orientation. The agreement between experimental [8111] and predicted [212]

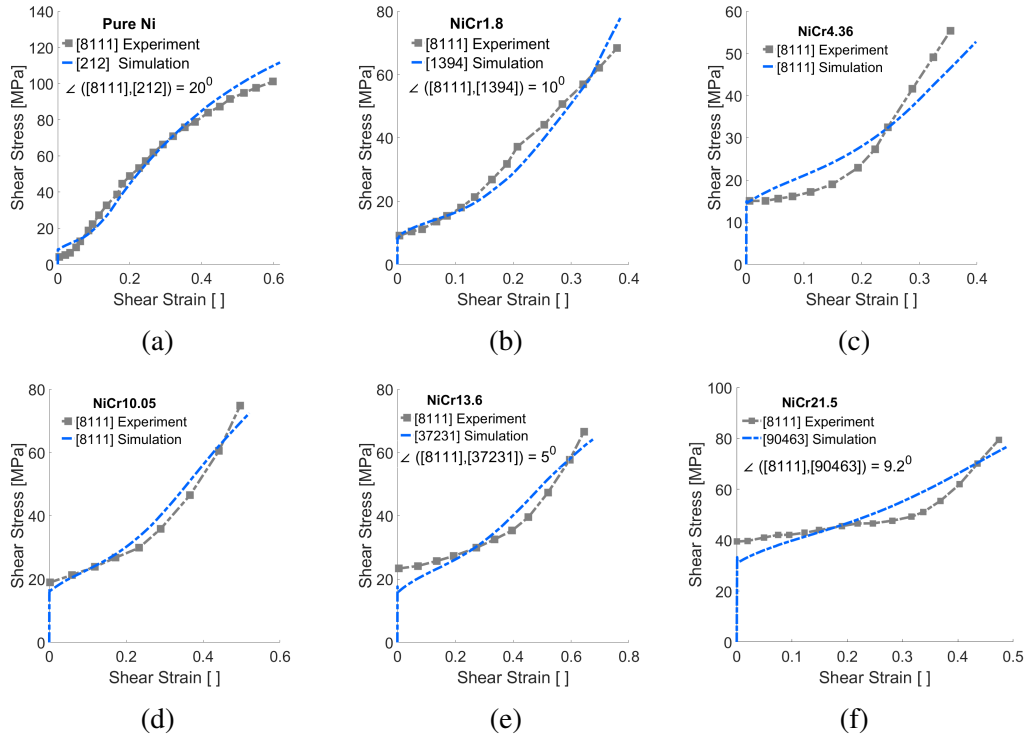


Figure 7.6: Prediction of stress strain curves of a) Pure Ni by 20° misorientation, b) NiCr1.8 by 10° misorientation and $s_0^t = 30.0$ MPa, c) NiCr4.36 by $s_0^t = 40.0$ MPa, d) NiCr10.05 by $s_0^t = 45.0$ MPa, e) NiCr13.6 by 5° misorientation and $s_0^t = 45.0$ MPa and f) NiCr21.5 by 9.2° misorientation and $s_0^t = 80.0$ MPa. The judgment about the possible experimental error is being done by both macroscopic stress-strain response and mesoscale structure. All simulations was done with the same unique set of parameters in Table 5.3. Experiments from Ref [40].

Ni crystals (20° misorientation) in Figure 7.6a clarifies the likely error in the reported crystal orientation. The experimental mesoscale structure of NiCr polycrystal in Figure 7.7 verifies the simulations and the error considerations in Figure 7.6. All simulations were done with the same unique set of parameters in Table 5.3. The sensitivity to the misorientation varies for different crystals. For pure Ni crystal in Figure 7.6a, a 20° misorientation is required to predict macroscopic response and also mesoscale structure in Figure 7.7. However, the required misorientation for NiCr1.8, NiCr13.6, and NiCr21.5 are 10° , 5° and 9.2° , respectively. Different degrees of sensitivity to the misorientation demand a comprehensive analysis to determine which crystals are more sensitive.

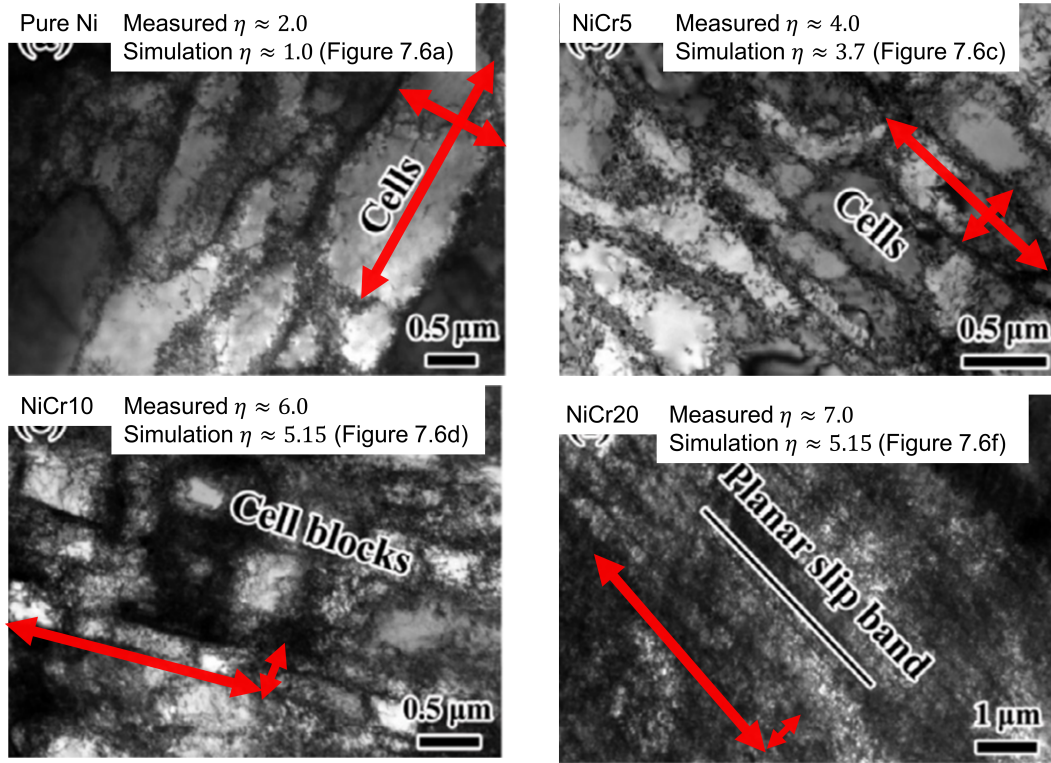


Figure 7.7: The experimental mesoscale structure of NiCr polycrystal that verifies the simulations and the error considerations in Figures 7.6. Experiments from Ref. [35].

The mesoscale structure stability and macroscopic response variability in misoriented crystals depend on the original crystal orientation. We repeated the crystal orientation sensitivity analysis for different crystals. Figure 7.8 demonstrates the sensitivity of crystals with $0 - 20^\circ$ misorientation from [100], [110], and [111] Ni crystals (most area of the inverse pole figure is covered). The uniform curves in the crystals with $0 - 5^\circ$ misorientation from [110] crystal in Figures 7.8a and 7.8d are due to stable Type-II structure. The stable structure in [100] and [111] crystals are equiaxed cells (Type-III). The postponed equiaxed cell formation by deviation from the original orientations shifts the stress-strain curves to the left in Figures 7.8b and 7.8c and produces stress variability. Type-I and II structures remain stable (without transformation to Type-III) for some crystals with more deviations ($0 - 10^\circ$). Different stable structures for crystals with $0 - 10^\circ$ misorientation produce noticeable stress variability (Figures 7.8e and 7.8f). The variability is more extensive for crystals in the neighborhood of [111]. By increasing the misorientation to

$0 - 20^\circ$, structure transformation occurs for more crystals. Stress variability due to structure variability for all three cases is apparent in Figures 7.8g, 7.8h, and 7.8i. As a result, stress-strain behavior differs for all crystals with considerable misorientation. Therefore, it is important to take caution when measuring orientation in the experiments. Crystals close to $[111]$ require a high degree of measuring accuracy due to their extreme sensitivity to misorientation. Even less than 10° misorientation may result in significant errors in stress-strain response.

7.2 Implications

Predictive power of a model in different conditions relates how the common linkage between predicted behaviour and its reason is employed. This linkage is between mechanical response and mesoscale dislocation substructures in FCC metals. We developed a crystal plasticity model to predict monotonic response based on substructures. Various substructures form in different applied strain ranges and crystal orientations that make it possible to parametrise substructures independently. The independent estimation of model parameters enabled us to propose a new crystal plasticity parameter optimisation. Optimised parameters for one FCC metal are applicable to predict other FCC metals behaviour due to common substructures in different FCC metals. Material invariant parameters are valuable for blind prediction of new materials with no experimental data. A robust model with optimised parameter to predict monotonic response guarantee right prediction of overload response in cyclic loading.

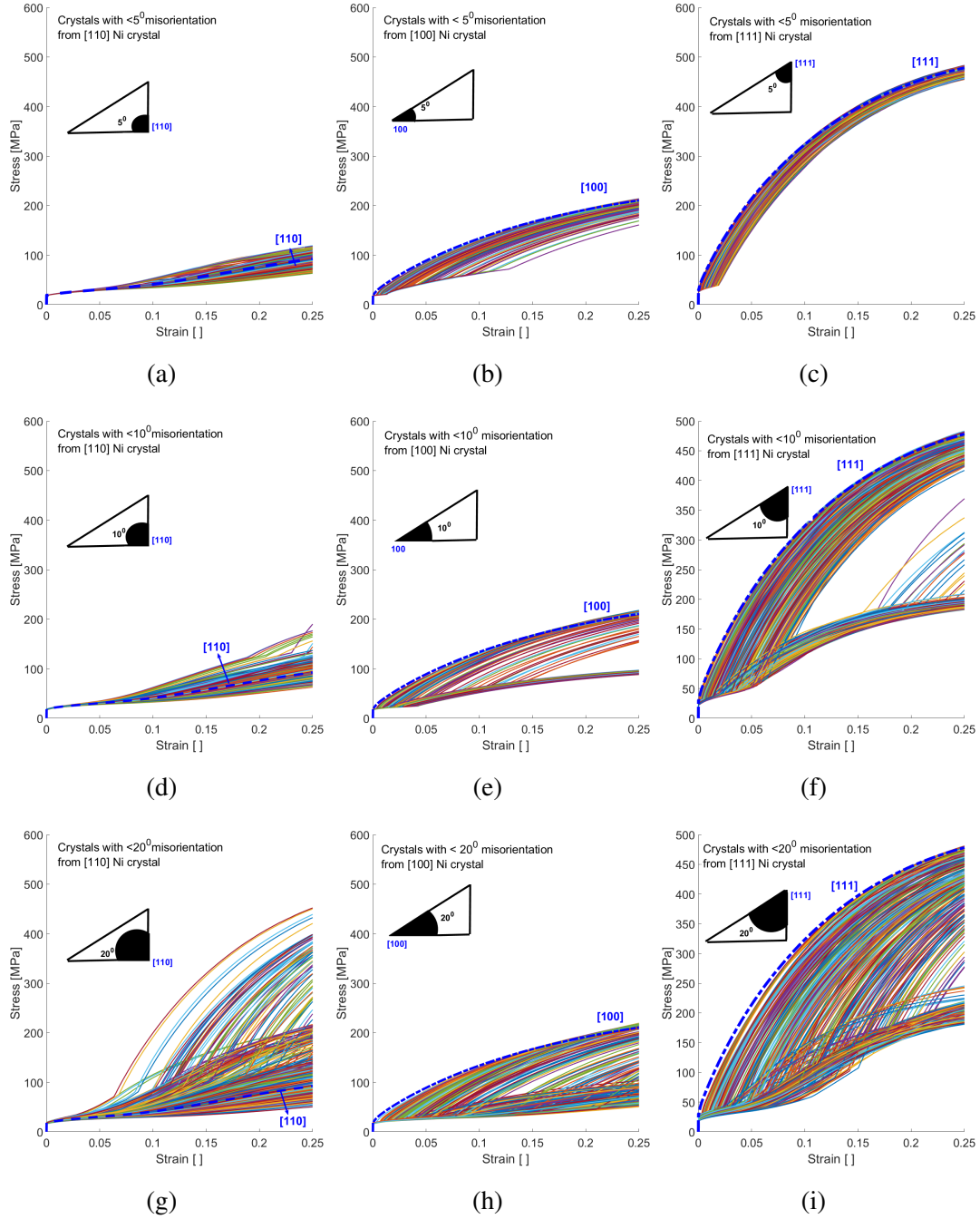


Figure 7.8: Orientation sensitivity of stress strain curves in different areas of inverse pole figure.

Chapter 8

Conclusions and Future Work

8.1 Conclusions

The first objective of this work was achieved by detailed analysis of the linkage between mesoscale substructures and macroscopic behaviour of FCC materials. Substructure attributes that control the macroscopic response is explained in crystal plasticity models constitutive equation.

We fulfilled **second objective** by implementing crystal plasticity model to predict not only macroscopic behaviour but also mesoscale structures of FCC metals in monotonic loading. Multiscale validation and verification with experiments show trustable prediction strategy. We compared the prediction power of our model with other crystal plasticity formulations and showed robust predictions.

Estimation of several parameters is key aspect of crystal plasticity models. Structural nature of model parameters in our model enabled us to achieve **third objective** by proposing a new sequential physics based parameter optimisation method. Parameters are estimated independently with minimum available experimental data, excellent fitting quality and with bounded uncertainty. Since structures are common among FCC metals, optimised model parameters are material invariant, i.e. parameters of one FCC metal are applicable to predict other FCC metals behaviour. This aspect enables blind predictability for new FCC metals without experimental data. We predicted the stainless steels behaviour with the parameters optimised by Cu experimental data.

We found in literature that effects of overloads during cyclic loading are defined by mesoscale dislocation substructures. Hence, **fourth objective** achieved by integrating substructure sensitive monotonic model with optimised parameters and cyclic model to predict the effect of overloads based on substructures. We predicted overload responses for Cu and NiCr single and poly-crystals by right mesoscale substructures. The model is applicable for blind prediction of any new FCC metal without single crystals experimental data.

8.2 Future Work

Mesoscale structures control the macroscopic stress-strain response by defining internal stresses (back and athermal stresses in Equations (3.20) and (4.12)). According to experiments [24], the structures at large grains (>250 micron) and single crystals are comparable. Hence, the effect of grain size and boundaries are not considered in this work, and the model is applied for single crystals and large-grain polycrystals. We also argue that plasticity is mainly controlled by grain interior structures in large grains. The plasticity mechanism, and internal stresses near the boundaries, are mainly formulated by strain gradient and GNDs in the literature.

Since the measurement of GNDs is difficult and uncertain, we challenge the present gradient-based models that parametrize internal stress by GNDs. However, the measurement of mesoscale structure attributes from TEM images (wall spacing, aspect ratio, and wall fraction) is more trustable. Unknown structures and mechanisms near boundaries limit the application of this model for small-grain polycrystals. Structures near boundaries, and their development mechanism, could be analyzed in future works to consider grain size and boundary effects.

This work regulated the relation between 12 active slip systems and the developed mesoscale structures in FCC metals under uniaxial loading. Since the slip system activity is different in multiaxial loading, the expected mesoscale structures are required to be re-formulated in future works. The possible influence of new dislocation interactions (activated in multiaxial loading) on the mesoscale structures, must be considered to relate internal stresses to the macroscopic response. Due to the difficulties of the multiaxial loading of single crystals, the new model can be used to reveal unknown mechanisms under multiaxial loading.

Two internal stresses are considered in this work, the back and athermal stress. While the back stress is defined by structure walls fraction, the athermal stress relates to cells' interior, i.e., dislocation mean free path and wall spacing. Therefore, The effects of wall fraction and aspect ratio can be exchanged. In other words, a unique value for macro-

scopic stress is achievable by large back (thick walls) and small athermal stress (long structure) or vice versa. Hence, further efforts should be done to decouple back and athermal stresses to provide a more explicit relation between the substructures and macroscopic stress-strain response.

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