

Revealing plastic strain heterogeneity and internal stresses in metallic alloys: insights from crystallographic texture

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Thesis typescript submitted in partial fulfilment of the requirements
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Revealing plastic strain heterogeneity and internal stresses in metallic alloys: insights from crystallographic texture

by Guillaume Hanon

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iMMC

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*“Ever tried. Ever failed. No matter.
Try again. Fail again. Fail better.”*

— SAMUEL BECKETT

“Ik moet just niks!”

— WOUT VAN AERT

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La science avance rarement de manière isolée, et une thèse en est sans doute la meilleure preuve. Il en a d'ailleurs toujours été ainsi. En 1675, Sir Isaac Newton écrivait déjà: *"If I have seen further it is by standing on the shoulders of giants"*. Bien que, historiquement, cette phrase puisse avoir plusieurs interprétations, cette métaphore résonne profondément avec mon état d'esprit à l'issue de ces quatre années. Car si l'aboutissement de cette thèse a exigé de longues heures de travail solitaire, celle-ci n'aurait jamais pu voir le jour sans le soutien d'un entourage de qualité. Je tiens donc à témoigner ma gratitude et à souligner l'importance de toutes les personnes qui m'ont permis de mener ce projet à son terme.

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Abstract

This work investigates plastic deformation heterogeneity at the macroscopic and microscopic scales within metallic alloys. Indeed, reaching a deeper understanding of the origins and consequences of heterogeneity is crucial, given its influence on the overall mechanical performance of the material.

The main originality of the approach is to use crystallographic texture to reveal and predict the development of non-uniform internal stresses and strain fields. This requires employing reliable crystal plasticity (CP) numerical models to relate the rotations of crystal lattices to the plastic deformation.

Three complementary studies are conducted to assess the validity of the approach. In extruded aluminum alloys, we find that the presence of texture gradients leads to the development of non-negligible internal stresses; incorporating initial texture data into CP models enables accurate prediction of both the magnitude and spatial distribution of these stresses during subsequent processing. In roll-bonded aluminum-steel multilaminates, texture analysis provides valuable insights into the macroscopic through-thickness strain distribution arising during successive roll-bonding passes. Finally, using CP based finite element modeling (CPFEM), we investigate how crystalline interfaces influence plastic strain heterogeneity at the grain scale. In this context, a novel CPFEM framework accounting for grain interactions across crystalline interfaces is proposed to better capture the local strain field when using non-conformal FE meshes.

List of Publications

Supporting publications

- **Hanon, G.**, Malet, L., Delannay, L., Texture and Microstructure After Roll-Bonding of an Fe-Al Multilaminate, Proceedings of the 14th International Conference on the Technology of Plasticity, 2024.
- **Hanon, G.**, Malet, L., Delannay, L., Heterogeneity of strain and texture inside roll-bonded multilaminates, Materials Research Proceedings, 2024
- **Hanon, G.**, Delannay, L., Modeling the influence of crystalline interfaces on the microscopic strain heterogeneity (in preparation)
- **Hanon, G.**, Pot, C., Bocher, P., Delannay, L., How heterogeneous plastic anisotropy in extruded AA6063 induces residual stresses (in preparation)

Communications in conference

- **Hanon, G.**, Delannay, L., FE modeling of the microscopic strain heterogeneity along grain boundaries, *12th European Solid Mechanics Conference (ESMC)*, Lyon, France.
- **Hanon, G.**, Delannay, L., Texture heterogeneity inside a roll bonded Fe-Al multilaminate subjected to plastic instabilities, *20th International Conference on Textures Of Materials (ICOTOM)*, Metz, France.
- **Hanon, G.**, Malet, L., Delannay, L., Heterogeneity of strain and textures inside roll-bonded multilaminates, *27th International ESAFORM Conference on Material Forming*, Toulouse, France.
- **Hanon, G.**, Malet, L., Delannay, L., Texture and microstructure after roll-bonding of an Fe-Al multilaminate, *14th International Conference on the Technology of Plasticity (ICTP)*, Mandelieu-La Napoule, France.
- **Hanon, G.**, Malet, L., Delannay, L., Refined modeling of the interaction of adjacent grains inside a Tungsten polycrystal, *ECCOMAS Young Investigators Conference YIC2023*, Porto, Portugal.

- **Hanon, G.**, Delannay, L., Toward the understanding of the interplay of plasticity and Hydrogen diffusion in rolled Aluminum, *9th International and multidisciplinary Summer School on hydrogen*, Besançon, France.

Table of abbreviations

α -fibre	Crystallographic fibre with $\langle 110 \rangle$ aligned with the rolling direction in BCC metals
β -fibre	Crystallographic fibre developed during rolling of FCC metals
γ -fibre	Crystallographic fibre with $\langle 111 \rangle$ aligned with the normal direction
$\bar{R}$	Normal anisotropy coefficient
ΔR	Planar anisotropy coefficient
b^α	Slip direction on slip system α
C_{11}, C_{12}, C_{44}	Elastic stiffness constants
D	Strain rate tensor
F	Deformation gradient tensor
$f(\sigma_{ij})$	Yield function
$\dot{\epsilon}_p$	Plastic strain rate tensor
$\dot{\epsilon}_{eq}$	Equivalent strain rate
$\dot{\gamma}^\alpha$	Shear rate on slip system α
$\dot{\gamma}_0$	Reference shear rate for the viscoplastic exponential law
$\dot{\gamma}_{rlx}$	Shear rate on fictitious slip system
$\{hkl\}\langle uvw \rangle$	Miller indices
J_2	Second invariant of the deviatoric stress tensor
l_c	Contact length between roll and sheet
L	Velocity gradient tensor
m	Strain-rate sensitivity exponent for the viscoplastic exponential law
M^α	Schmid tensor
μ	Friction coefficient or shear modulus
n^α	Normal direction to slip plane α
Ω	Computational domain
Ω^*	Lattice spin tensor
q -value	Anisotropy coefficient derived from Lankford coefficient
q_0, q_1, q_2, q_3	Quaternion components
$R\psi$	Lankford coefficient for loading at angle ψ
R^*	Lattice rotation tensor
s	Deviatoric stress tensor
$\sigma_{yield}(\psi)$	Uniaxial plastic yield stress for loading at angle ψ
$\frac{\sigma_{yield}(\psi)}{\sigma_{yield}(90^\circ)}$	Flow stress ratio
σ	Cauchy stress tensor

T	Second Piola-Kirchhoff stress tensor
τ^α	Resolved shear stress on slip system α
τ_c^α	Critical resolved shear stress
$\tau_{c0}, \Gamma_0, n, K, \sigma_{y,0}$	Hardening parameters (Swift law)
U	Stretch tensor
W	Spin tensor
W_{el}	Elastic strain energy
$\dot{W}$	Plastic work rate
$\varphi_1, \Phi, \varphi_2$	Euler angles
ψ	Angle between tensile and reference directions
BCC	Body-centred cubic
CG	Centre of the grain
CP	Crystal plasticity
CPFEM	Crystal plasticity finite element model
CRSS	Critical resolved shear stress
DIC	Digital image correlation
ED	Extrusion direction
EBSD	Electron backscatter diffraction
FCC	Face-centred cubic
FE	Finite element
GB	Grain boundary
GNDD	Geometrically necessary dislocations density
KAM	Kernel average misorientation
M	Taylor factor
ND	Normal direction to the rolling plane
ODF	Orientation distribution function
PF	Pole figure
QP	Quadruple point
R	Lankford coefficient (R-value) or radius of curvature
RD	Rolling direction
S	Normalized through-thickness position
SFE	Stacking fault energy
TD	Transverse direction in a rolled plate
Taylor FC	Taylor full-constraint
Taylor RC	Taylor relaxed-constraint
th	Thickness of the specimen
TJ	Triple junction
VM	Von Mises
XRD	X-ray diffraction

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Introduction

| 1

Technological development continues to accelerate in an increasingly interconnected world, permeating nearly all aspects of modern life. Nowadays, this rapid evolution is driven not only by societal demand for efficiency and performance, but also by the urgent need to mitigate global warming and improve safety. These last challenges motivate the scientific community to continue to push the boundaries of current knowledge in all the engineering domains to design cleaner, safer and more reliable technologies.

In materials mechanics, the pursuit of higher ductility, strength, and toughness pushes researchers to investigate the heterogeneous stress and strain fields that develop within metallic materials. These heterogeneities may arise across multiple length scales, from intragranular variations within polycrystalline aggregates to macroscopic gradients across the thickness of structural components. Such non-uniform deformation and stress states may trigger strain localization and damage initiation, thereby exerting a decisive influence on material performance and failure. A deeper understanding of these heterogeneous fields is therefore essential for the design and optimization of metal alloys as well as metal-forming processes.

Measurements of stresses and plastic strains in the bulk of metallic alloys are experimentally challenging. It is much easier to probe the deformation-induced crystallographic texture.

The main objective of this thesis is to predict and reveal heterogeneous stress and plastic strain fields in a metal alloy by exploiting crystallographic texture in an original way.

This thesis is structured into five chapters:

Chapter 2 presents the theoretical framework required to understand the manuscript and to clearly define the research questions that motivated this thesis.

Chapter 3 characterizes the plastic anisotropy associated with the distinct

texture measured in extruded aluminium alloys investigates the development of internal stresses arising from the interaction between layers with contrasting textures. This chapter combines experimental observations and crystal plasticity simulations to provide a comprehensive understanding.

Chapter 4 explores the development of strain heterogeneity through the thickness of multilayers produced by roll bonding, using crystallographic texture. A numerical framework is presented to enable the interpretation of experimentally measured texture gradients in terms of through-thickness strain heterogeneity.

Chapter 5 characterizes the heterogeneity of the microscopic deformation field within a polycrystal and assesses the key features of grain interactions across crystalline interfaces. An original approach for incorporating these interactions into a CPFEM framework is also presented

Conclusions are provided at the end of each chapter, while the global conclusions and perspectives are presented in **Chapter 6**.

Basics of the interplay between plasticity and texture

2

This chapter introduces the theoretical foundations necessary for the comprehension of the manuscript.

The chapter is organized as follows. Section 2.1 reviews the definition and characterization of crystallographic texture, a central concept throughout this work. Section 2.2 presents the different approaches used to model plastic response and examines their ability to account for the influence of texture. Subsequently, the crystal plasticity models employed in this study are presented in Section 2.3, where the hypotheses linking micro-scale plastic deformation to the macroscopic response are developed. The derivation and the numerical implementation of the governing crystal plasticity equations is provided in Section 2.4. Finally, Section 2.5 outline the specific objectives of the thesis.

2.1 How does plasticity induce crystallographic texture in metals?

In most industrial applications, metals have polycrystalline microstructures consisting of an aggregate of grains, each characterized by a specific crystallographic orientation. When certain orientations occur more frequently than others, the material is said to exhibit a texture. Conversely, a random texture denotes the absence of any preferential orientation.

The crystallographic orientation of a grain is commonly described using the three Euler angles $(\varphi_1, \Phi, \varphi_2)$, which define the transformation from the specimen coordinate system (X, Y, Z) to the crystal coordinate system (x, y, z) , whose axes coincide with the crystallographic directions $([100], [010], [001])$. These angles are applied in a prescribed rotation sequence: φ_1 is a rotation about Z -axis, Φ is a rotation about the intermediate X' -axis and φ_2 is a rotation about the final z -axis (Figure 2.1.a). Each triplet $(\varphi_1, \Phi, \varphi_2)$ defines a point in the 3D Euler space, bounded by $([0, 2\pi] \times [0, 2\pi] \times [0, 2\pi])$. However, crystal

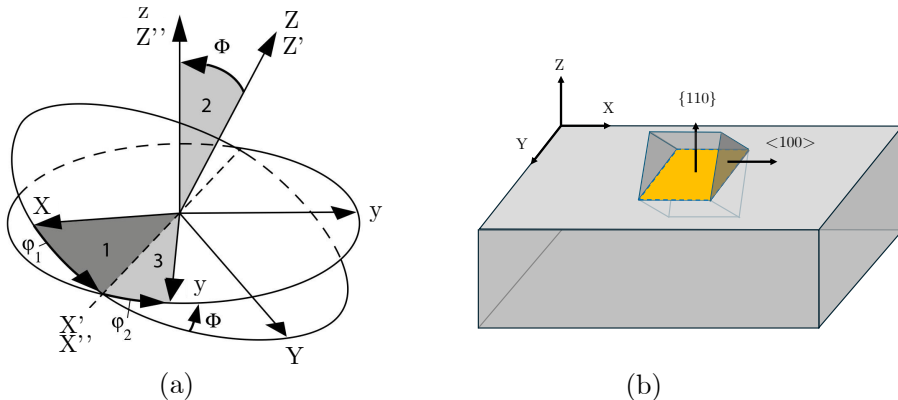


Figure 2.1: (a) Illustration of the rotation sequence using the three Euler angles ($\varphi_1, \Phi, \varphi_2$) to transform from the specimen reference frame (X, Y, Z) to the crystal reference frame (x, y, z). (b) Representation of a crystal orientation using Miller indices, where $\langle uvw \rangle$ indicates the crystal direction aligned with the specimen X -axis, and $\{hkl\}$ indicates the crystal plane normal aligned with the specimen Z -axis. Figures are reproduced and adapted from Engler and Randle (2009).

and sample symmetries enable to reduce significantly the size of the space to define univocally every possible crystallographic orientations. For metals having a cubic structure (such as those studied in this work), crystal symmetry reduces the fundamental region to $\Phi \in [0, \pi/2]$ and $\varphi_2 \in [0, \pi/2]$. Furthermore, in plane-strain deformation conditions, such as rolling, the orthonormal sample symmetry allows reduction of $\varphi_1 \in [0, \pi/2]$.

Crystallographic orientations may also be expressed using Miller indices. An orientation denoted as $\{hkl\}\langle uvw \rangle$ indicates that the crystal direction $\langle uvw \rangle$ is aligned with the specimen X -axis, while the direction $\{hkl\}$ is parallel to the specimen Z -direction (Figure 2.1.b). This notation provides a direct and intuitive link between crystal directions and specimen axes, making it particularly suitable for describing ideal texture components.

A classical way to visualize the distribution of orientations in a polycrystal is the pole figures. They provide a representation of the probability that a given crystallographic plane is normal to a particular spatial direction. They are constructed by determining the intersections between the normals to selected crystallographic planes (such as $\{100\}$, $\{110\}$, or $\{111\}$) and the surface of a sphere, followed by stereographic projection of these intersections onto a two-dimensional plane. This projection plane is defined by the specimen reference frame, typically associated with the deformation axes. For rolled

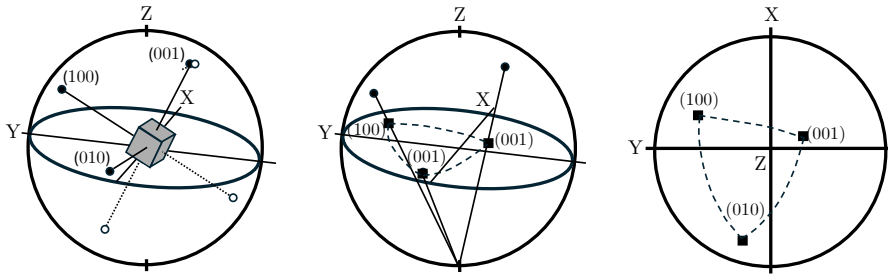


Figure 2.2: Schematic of the stereographic projection of the 100 axes of a cubic crystal onto the XY-plane to construct the $\{100\}$ pole figure. This procedure is repeated for all grains in the polycrystal to obtain the overall texture. This figure is a reproduction from Engler and Randle (2009).

sheets, for instance, the projection plane is commonly defined by the rolling direction (RD) and transverse direction (TD). Figure 2.2 illustrates the stereographic projection of the $\{100\}$ axes of a cubic crystal onto the XY-plane to construct the corresponding pole figure. Repeating this procedure for all grains in the aggregate gives the representative pole figure that characterizes the crystallographic texture of the polycrystal.

Pole figures are particularly effective for characterizing fibre textures, which consist of sets of crystallographic orientations generated by rotating a crystal around a fixed axis. A representative example is the texture developed during uniaxial tension of FCC metals, illustrated in Figure 2.3. The $\{111\}$ pole figure reveals a pronounced concentration of crystals whose $\langle 111 \rangle$ axes are aligned with the tensile direction (X-direction). In contrast, the $\{100\}$ pole figure displays two rings with high intensities located symmetrically with respect to the Y-axis. This combination of characteristics corresponds to a set of grains whose $\langle 111 \rangle$ axes coincide with the loading direction while differing only by rotations around the X-axis (Figure 2.3.c). Such an orientation set constitutes a classical fibre texture. In this context, pole figures alone provide an unambiguous and sufficiently complete representation of the underlying crystallographic texture. Fibre textures are typically produced by uniaxial deformation processes such as tension/compression, wire drawing and extrusion

For deformation processes involving more complex strain paths, such as the plane-strain compression imposed during rolling, pole figures alone are often insufficient for an unambiguous interpretation of the texture. As illustrated in Figure 2.4.a and .b, the $\{111\}$ and $\{100\}$ pole figures of a rolled FCC metal reveal a texture that is much more difficult to interpret than those associated with simple fibre textures. Moreover, pole figures may lead to ambiguity because

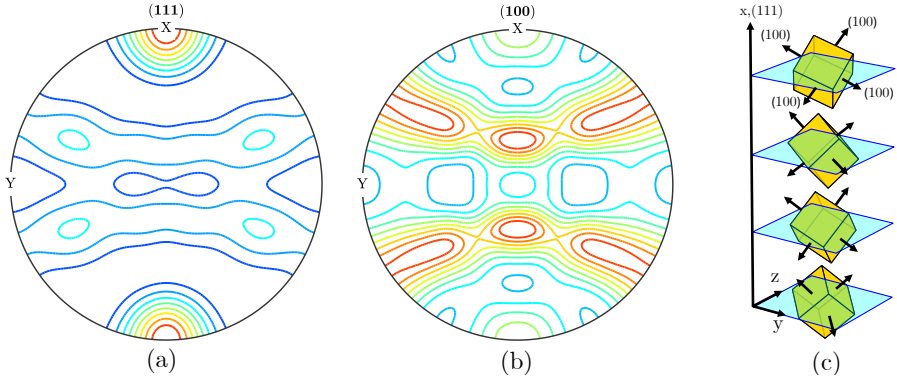


Figure 2.3: Illustration of the texture of an FCC metal deformed by traction using (a) Pole figure representing $\{111\}$ poles projected on the plane defined by the tensile direction (X) and transverse direction (Y) (b) Pole figure representing $\{100\}$ poles projected on the plane defined by the tensile direction (X) and transverse direction (Y) (c) Schematic representation of a collection of grains whose $\{111\}$ planes are aligned with the tensile axis, while their $\{100\}$ planes differ by rotations around the X-axis.

the individual components cannot be clearly identified. Indeed, as previously discussed, three Euler angles are required to uniquely define a crystallographic orientation, meaning that the natural space for texture representation is three-dimensional. Projecting this 3D distribution of orientations onto a 2D plane inevitably results in a loss of information, as distinct orientations may overlap in the same pole figure. The Orientation Distribution Function (ODF), $f(g)$, overcomes this limitation by providing a complete statistical description of texture by expressing the probability density of orientations within Euler space:

$$\text{odf}(g) = f(g) = \frac{1}{V} \frac{dV(g)}{dg} \quad (2.1)$$

where V is the specimen volume and $dV(g)$ the volume of material having orientation g . Figures 2.4.c–e show sections of the ODF for the rolled sheet at several values of φ_2 , highlighting the main crystallographic orientations developed during rolling. The ODF enables a clear identification of crystallographic orientations and allows texture to be characterized in different ways: by the volume fraction of ideal texture components, by the volume fraction of grains having orientations belonging to the same fibre or by the evolution of the orientation density along a fibre.

The orientations of individual crystals within a specimen can be measured using X-ray diffraction (XRD), neutron diffraction, or electron backscatter diffraction (EBSD). In this work, all the texture measurements were obtained using EBSD, and the pole figures and ODFs were processed using the MTEX

toolbox (Hielscher and Schaeben, 2008).

Different physical mechanisms can be at the origin of the development of crystallographic texture in a polycrystal. In the present work, we consider exclusively the texture induced by dislocation slip. Unlike mechanical twinning, which produces an abrupt lattice reorientation across the twinning plane, dislocation slip leads to progressive and continuous rotation of the crystal lattice.

Figure 2.5 illustrates the lattice rotation of a single crystal subjected to uniaxial tension. In this configuration, elongation of the crystal could, in theory, be achieved while activating only one slip system. Although simple shear kinematics would predict a rotation of the material line away from the loading axis, experimental observations demonstrate that this line remains aligned with the principal loading direction (Hosford, 2010). This discrepancy is resolved by the fact that the lattice undergoes an intrinsic rotation, described by a rotation tensor, $\mathbf{R}^*$, which counterbalances the rotation induced by slip.

When multiple slip systems are simultaneously activated, each one contributes to the overall lattice rotation. If the combined effect of these contributions results in a net rotation $\mathbf{R}^* = 0$, the crystal has reached a stable orientation. This situation is illustrated in Figure 2.6.

In a polycrystalline aggregate, plastic deformation is accompanied by the development of crystallographic texture due to the progressive reorientation of the lattice in each grain. As plastic strain increases, grains gradually rotate toward their corresponding stable orientations, and the volume fraction of grains reaching these orientations increases accordingly.

In Chapter 4, we investigate the textures produced by cold rolling. It is therefore useful to have a brief introduction about the typical rolling textures developed in FCC and BCC metals and the parameters influencing them. Table 2.1 summarizes the principal texture components and fibres.

In FCC metal, rolling generally produces β -fibre (linking the Copper, S, and Brass components) and partial α -fibre (from Brass to Goss) (Kocks et al., 2000). However, despite sharing the same fibre components, rolling can lead to two distinct types of textures: the typical *copper-type texture* (also referred to as the *pure-metal-type texture*), which is mainly composed of the Copper, S, and Brass components, and the *brass-type texture* (or *alloy-type texture*), which is dominated by the Brass component. Intermediate texture, representing a mixture of both types, have also been reported (Hirsch and Lücke, 1988). The transition between these texture types arises from the combined effects of the stacking fault energy (SFE) (Stephens, 1968; Hu, 1974; Hirsch and Lücke, 1988; Ray, 1995; Dillamore and Roberts, 1965) and the rolling temperature (Hu and Cline, 1961; Hu, 1974). In this work, aluminium alloys having a high

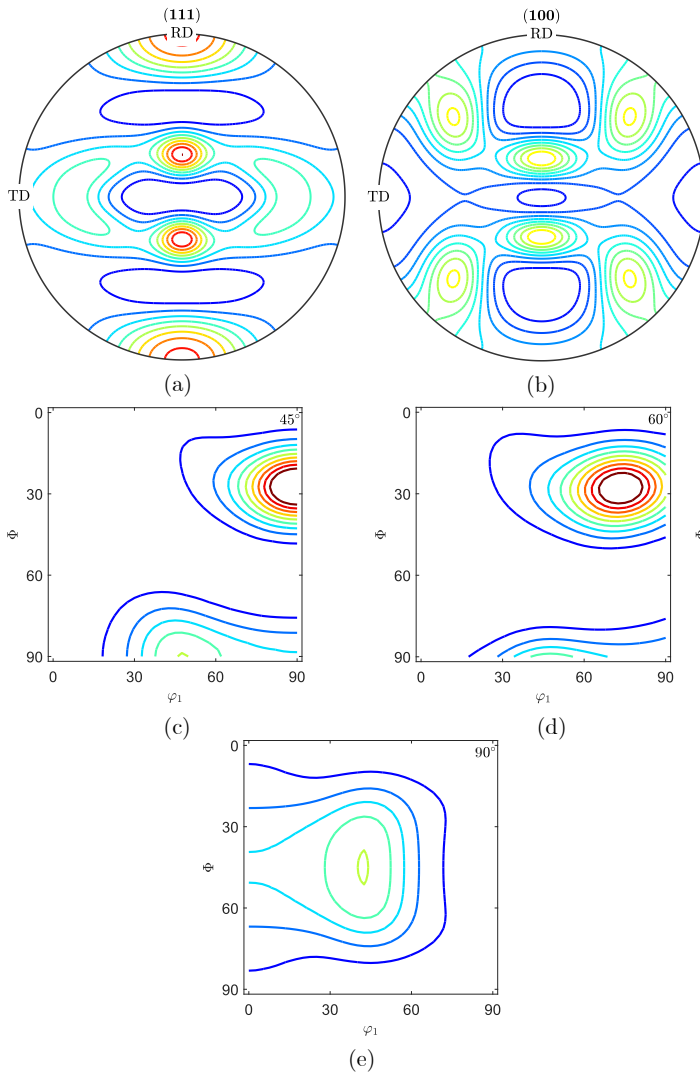


Figure 2.4: Illustration of texture development in an FCC metal subjected to plane-strain compression (rolling): (a) $\{111\}$ pole figure projected on the plane defined by the rolling direction (RD) and transverse direction (TD) (b) $\{100\}$ pole figure projected on the plane defined by the rolling direction (RD) and transverse direction (TD) (c–e) Sections of the orientation distribution function (ODF) at $\varphi_2 = 45^\circ$, 60° , and 90° , highlighting the main crystallographic orientations developed during rolling.

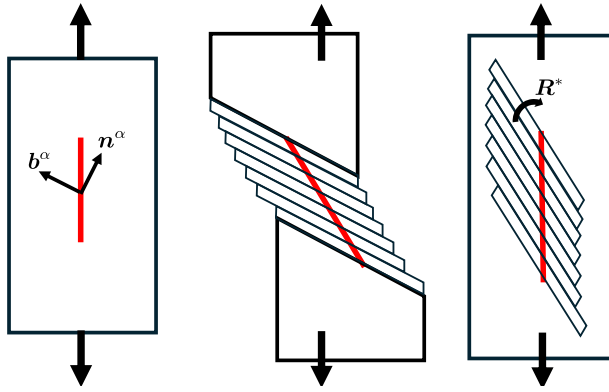


Figure 2.5: Progressive lattice rotation induced by dislocation glide under uniaxial loading. The lattice rotation maintains the material line fixed during deformation. Here, b^α and n^α denote the slip direction and slip plane normal, respectively, and R^* is the rotation tensor associated with lattice rotation contributing to texture development.

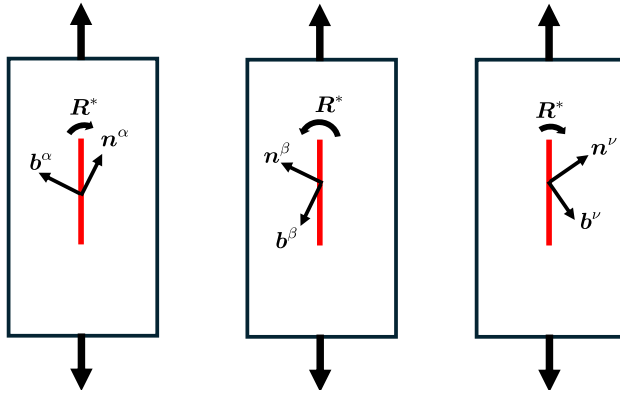


Figure 2.6: Illustration of the combined effect of multiple slip systems on lattice rotation. Slip along different planes (α, β, ν) with slip directions b and slip plane normals n can result in a net lattice rotation of $\sum R^* = 0$, corresponding to a stable crystal orientation.

	$\{hkl\}\langle uvw \rangle$	$\varphi_1, \Phi, \varphi_2$
α (FCC)	$\langle 110 \rangle // \text{ND}$	
α (BCC)	$\langle 110 \rangle // \text{RD}$	
β		
γ	$\langle 111 \rangle // \text{ND}$	
Copper	$\{112\}\langle 111 \rangle$	$90^\circ, 35^\circ, 45^\circ$
S	$\{123\}\langle 634 \rangle$	$59^\circ, 37^\circ, 63^\circ$
Goss	$\{011\}\langle 100 \rangle$	$0^\circ, 45^\circ, 90^\circ$
Brass	$\{011\}\langle 211 \rangle$	$35^\circ, 45^\circ, 90^\circ$
Cube	$\{001\}\langle 100 \rangle$	$0^\circ, 0^\circ, 0^\circ$

Table 2.1: Principals fibres and texture components identified in FCC and BCC metals rolled.

stacking-fault energy (SFE) are investigated, meaning that only copper-type textures are studied. It is also noteworthy that increasing the rolling reduction ratio generally sharpens the texture and slightly shifts the peak positions (Kestens and Pirgazi, 2016; Kocks et al., 2000).

In BCC metals, rolling promotes the development of the γ -fibre (running from $\{111\}\langle 110 \rangle$ to $\{111\}\langle 112 \rangle$) and a partial α -fibre (from $\{001\}\langle 110 \rangle$ to $\{111\}\langle 110 \rangle$) (Kestens and Pirgazi, 2016). Unlike FCC metals, the evolution of rolling textures in BCC metals is largely insensitive to solute additions (Ray et al., 1994; Ashby et al., 1999).

For rolling, ODF sections at $\varphi_2 = 45^\circ$ are often analysed, as many key texture components (α -fibre, γ -fibre, Copper, Brass and Goss components) are located in this section. The main texture components and fibres used to describe rolling textures in FCC and BCC metals are shown in Figure 2.7. Pole figure and ODF illustrating the texture of a FCC metal rolled are presented in Figure 2.4.

2.2 How does texture induce plastic anisotropy in metals?

Plasticity theory is essential for predicting material yielding under complex stress states and for determining the associated deformation, both of which are critical for the development of safe and reliable engineering technologies. Typical applications include the assessment of crashworthiness and impact response of automotive components, the design of aerospace structural parts formed by stamping and the evaluation of the mechanical properties of pre-strained metallic sheets. Furthermore, as discussed in the previous section, plastic deformation is intrinsically linked to the development of crystallographic texture. A robust theoretical framework for plasticity is therefore also

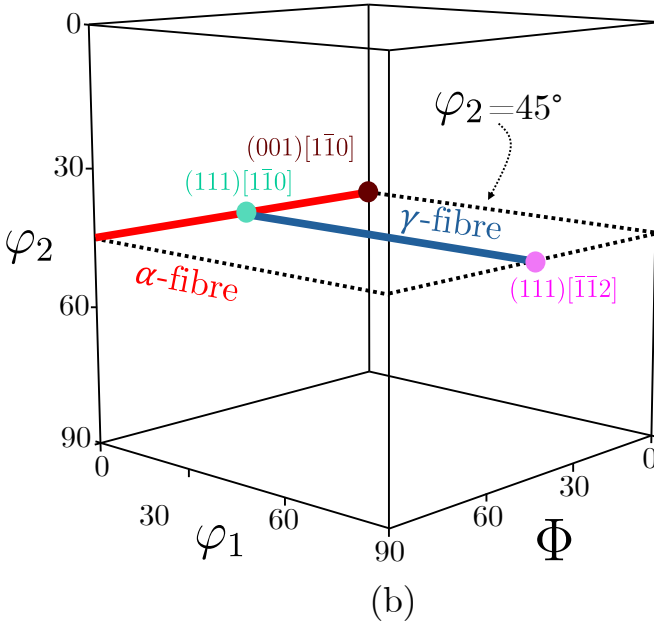
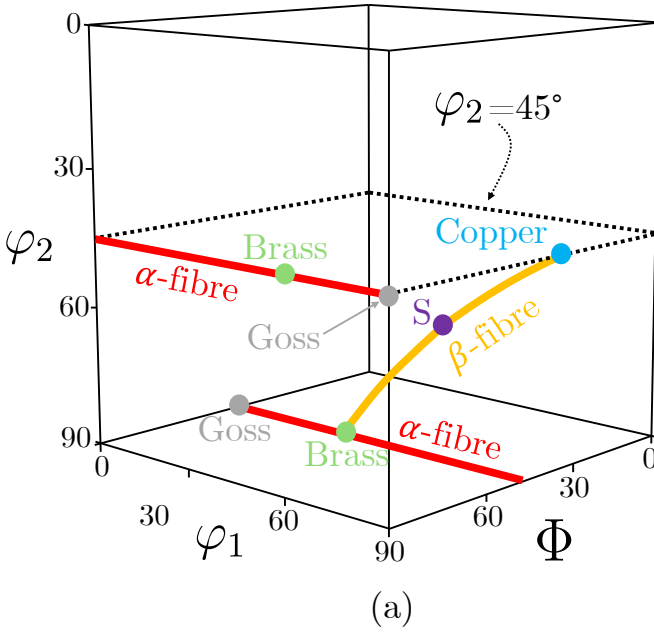


Figure 2.7: Locus of orientation defining the different fibres necessary to describes the textures developed during cold rolling (a) in fcc metals and (b) in bcc metals. These figures are reproduced and adapted from Kestens and Pirgazi (2016).

required to describe and predict texture evolution in metals. For these reasons, numerous plasticity models have been proposed to capture the behaviour of materials subjected to complex loading paths.

The selection of an appropriate plasticity model typically relies on experimental data obtained from tensile tests conducted along different material directions. These tests provide both the stress required to initiate plastic yielding, denoted σ_{yield} , and the corresponding Lankford coefficient or R -value. For uniaxial tension in the x -direction, the Lankford coefficient is defined as the ratio of the in-plane transverse plastic strain rate to the through-thickness plastic strain rate:

$$R = \frac{\dot{\epsilon}_{yy}^p}{\dot{\epsilon}_{zz}^p} \quad (2.2)$$

Where $\dot{\epsilon}_{yy}^p$ and $\dot{\epsilon}_{zz}^p$ represent the plastic strain rates in directions perpendicular to the tensile axis. By definition, the Lankford coefficient can range from zero to large values, as there is no strict upper limit. In practice, R -values are measured along multiple in-plane orientations. For instance, in a rolled metallic sheet, Lankford coefficients are determined for tensile directions spanning from the rolling direction (RD) to the transverse direction (TD), with the sheet thickness corresponding to the normal direction (ND). In this context, $R\psi$ denotes the Lankford coefficient for a tensile axis inclined by an angle ψ relative to RD, while $R0$ and $R90$ correspond to measurements along the RD and TD, respectively.

Materials exhibiting in all directions $R = 1$ are considered isotropic. The most widely used model for isotropic plasticity is the $J2$ theory. Its formulation relies on the observation that plastic flow in metals is insensitive to hydrostatic pressure ($tr(\sigma)/3$) and occurs at constant volume (Banabic, 2000). Consequently, yielding is governed exclusively by the deviatoric stress tensor ($\mathbf{s} = \sigma - \frac{tr(\sigma)}{3}\mathbf{I}$). The isotropic von mises yield criterion assumes that plastic yielding occurs when the elastic strain energy W_{el} reaches a critical value (Mises, 1913). For any stress state, the corresponding elastic energy can be expressed as:

$$\begin{aligned} W_{el} &= \frac{1}{2} \mathbf{s} : \text{dev}(\boldsymbol{\epsilon}) \\ &= \frac{1}{2} \mathbf{s} : \frac{\mathbf{s}}{2\mu} \end{aligned} \quad (2.3)$$

where μ is the shear modulus and $\text{dev}(\boldsymbol{\epsilon})$ is the deviatoric part of the strain tensor. Uniaxial tensile tests are commonly used to determine the critical value of W_{el} , as they provide the stress at the onset of plastic yielding, σ_{yield} . For

such loading, the corresponding elastic energy immediately prior to yielding is $W_{el} = \frac{\sigma_{yield}^2}{6\mu}$. Accordingly, for any stress state applied to an isotropic material, plastic deformation occurs when:

$$W_{el} = \frac{1}{2} \mathbf{s} : \frac{\mathbf{s}}{2\mu} = \frac{\sigma_{yield}^2}{6\mu} \quad (2.4)$$

This condition defines the yield locus, which represents the set of stress states that initiate plastic flow. The von Mises yield criterion can be expressed as:

$$\begin{aligned} f(\sigma_{ij}) &= \frac{1}{2} [(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{yy} - \sigma_{zz})^2 + 6(\sigma_{xy}^2 + \sigma_{xz}^2 + \sigma_{yz}^2)] \\ &= \frac{3}{2} \mathbf{s} : \mathbf{s} = 3(J2) \\ &= \sigma_{eq}^2 \\ &= \sigma_{yield}^2 \end{aligned} \quad (2.5)$$

where $J2$ the second invariant of the deviatoric part of the stress tensor and σ_{eq} the equivalent stress. As the criterion depends only on $J2$, it is inherently isotropic. This model is therefore well suited for materials exhibiting nearly isotropic behaviour.

Yield criteria determine the onset of plasticity and are commonly coupled with an associated flow rule, or normality rule, according to which the plastic strain rate tensor is normal to the yield surface:

$$\dot{\epsilon}_p = \dot{\lambda} \frac{\partial f}{\partial \sigma} \quad (2.6)$$

Where $\dot{\epsilon}_p$ is the plastic strain rate tensor, $\dot{\lambda}$ is a plastic multiplier whose amplitude results from kinematics and f is the function describing the yield locus. Therefore, the associated flow rule for the von mises criterion gives:

$$\begin{aligned} \frac{\partial f}{\partial \sigma_{xx}} &= \frac{\partial \dot{\epsilon}_{xx,p}}{\partial \dot{\lambda}} = 2\sigma_{xx} - \sigma_{yy} - \sigma_{zz} \\ \frac{\partial f}{\partial \sigma_{yy}} &= \frac{\partial \dot{\epsilon}_{yy,p}}{\partial \dot{\lambda}} = 2\sigma_{yy} - \sigma_{xx} - \sigma_{zz} \\ \frac{\partial f}{\partial \sigma_{zz}} &= \frac{\partial \dot{\epsilon}_{zz,p}}{\partial \dot{\lambda}} = 2\sigma_{zz} - \sigma_{xx} - \sigma_{yy} \end{aligned} \quad (2.7)$$

For uniaxial tension along the x -direction ($\sigma_{yy} = \sigma_{zz} = 0$, $\sigma_{xx} \neq 0$) and along the y -direction ($\sigma_{xx} = \sigma_{zz} = 0$, $\sigma_{yy} \neq 0$), the corresponding R -values are

$$R0 = \frac{d\dot{\epsilon}_{yy,p}}{d\dot{\epsilon}_{zz,p}} = 1 \quad R90 = \frac{d\dot{\epsilon}_{xx,p}}{d\dot{\epsilon}_{zz,p}} = 1 \quad (2.8)$$

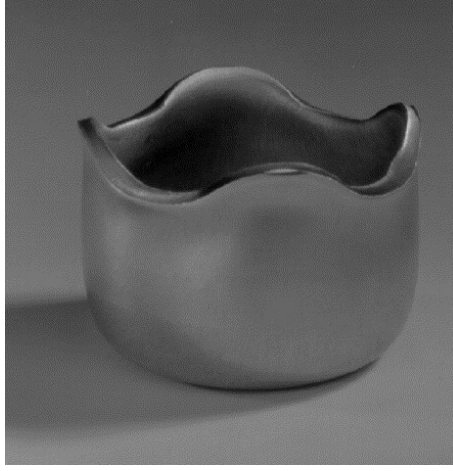


Figure 2.8: Development of ears on a cup produced by deep drawing of a textured aluminium sheet. This Figure is extracted from Engler et al. (2005).

These results confirm the suitability of the associated flow rule coupled with the von Mises criterion to predict isotropic plastic behaviour.

Many metallic materials deviate from isotropic plastic behavior, exhibiting so-called plastic anisotropy, where the plastic deformation response depends on the direction of the applied load. In metals, plastic anisotropy may arise from various factors, including crystallographic texture, preferred alignment of secondary phases and inclusions, dislocation structures, and average grain shape (Kocks et al., 2000; Delannay and Barnett, 2012; Alankar et al., 2014; Zubelewicz, 2021). A typical manifestation of this anisotropic behaviour is the formation of “ears” during the deep drawing of rolled aluminium sheets, such as those used in beverage can, as illustrated in Figure 2.8 (Engler, 2025). In such textured materials, the Lankford coefficient (R-value) varies with the loading direction relative to the rolling direction, leading to non-uniform thinning and, consequently, an inhomogeneous cup-wall height. In this work, we focus exclusively on cases where plastic anisotropy is induced by texture.

A famous anisotropic quadratic yield criterion was proposed by Hill. It accounts for orthotropic material symmetry (Hill, 1948). The Hill yield function can be written as:

$$2f(\sigma_{ij}) \equiv F(\sigma_{yy} - \sigma_{zz})^2 + G(\sigma_{zz} - \sigma_{xx})^2 + H(\sigma_{xx} - \sigma_{yy})^2 + 2(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2) = \sigma_{yield}^2 \quad (2.9)$$

The coefficients F, G, H, L, M, N are used to capture the anisotropy. These parameters are calibrated using 6 experimental measures. Note that setting all

coefficients equal to one recovers the isotropic von Mises criterion. Applying the associated flow rule to Hill yield criterion gives:

$$\begin{aligned}\frac{\partial f}{\partial \sigma_{xx}} &= \frac{\partial \dot{\epsilon}_{1,p}}{\partial \dot{\lambda}} = (G + H)\sigma_{xx} - H\sigma_{yy} - G\sigma_{zz} \\ \frac{\partial f}{\partial \sigma_{yy}} &= \frac{\partial \dot{\epsilon}_{2,p}}{\partial \dot{\lambda}} = (F + H)\sigma_{yy} - H\sigma_{xx} - F\sigma_{zz} \\ \frac{\partial f}{\partial \sigma_{zz}} &= \frac{\partial \dot{\epsilon}_{3,p}}{\partial \dot{\lambda}} = (F + G)\sigma_{zz} - G\sigma_{xx} - F\sigma_{yy}\end{aligned}\quad (2.10)$$

The corresponding Lankford coefficients are then:

$$R0 = \frac{d\dot{\epsilon}_{yy,p}}{d\dot{\epsilon}_{zz,p}} = \frac{H}{G} \quad R90 = \frac{d\dot{\epsilon}_{xx,p}}{d\dot{\epsilon}_{zz,p}} = \frac{H}{F} \quad (2.11)$$

showing clearly that $R0 \neq R90 \neq 1$ for anisotropic materials, as these values depend on the coefficients characterizing the plastic anisotropy.

Under plane stress conditions and assuming alignment of material axes and principal directions of the stress tensor, only 3 experimental measures are required for the calibration. However, three tensile tests provide three yield stresses and three Lankford coefficients, while only three parameters (F, G, H) must be calibrated. As a result, multiple sets of coefficients may be obtained depending on which subset of experimental data is used, and the calibrated yield locus captures only the selected data. To improve accuracy and flexibility, more advanced yield criteria involving additional coefficients have been proposed including Yld91 (Barlat et al., 1991), Yld2000-2D (plane stress) (Barlat et al., 2003), BBC family (Banabic et al., 2003, 2005), 12 coefficients yield locus (Bron and Besson, 2004) and Yld2004-18p (Barlat et al., 2005). While these models enhance predictive accuracy, they require additional experiments for calibration.

The macroscopic models presented above are phenomenological, constructed from experimental observations of macroscopic plastic behaviour. Although these models can capture anisotropy when their coefficients are properly calibrated, they do not account for the physical origins of plastic anisotropy. At the microscopic scale, each grain within a polycrystalline material exhibits highly anisotropic plastic behaviour, as dislocation glide is restricted to a discrete set of slip systems. In a polycrystal with a random texture, the microscopic anisotropy of individual grains averages out, and the material behaves approximately isotropically at the macroscopic scale. However, when a preferred crystallographic texture develops, certain orientations become more frequent, and the corresponding anisotropy appears in the macroscopic response. This effect is neglected by the macroscopic models

presented above. Moreover, these models are inherently unable to predict the evolution of texture during plastic deformation. In contrast, crystal plasticity theory accounts for the intrinsic anisotropic behaviour of individual grains, enabling predictions of both macroscopic plastic response and texture evolution.

Dislocation glide occurs along well-defined crystallographic planes and directions. Slip systems correspond to the most densely packed atomic planes along which dislocations can move and are commonly expressed using Miller indices as $\{hkl\}\langle uvw \rangle$, where here $\{hkl\}$ denotes the crystallographic axis normal to the slip plane and $\langle uvw \rangle$ the crystallographic axis aligned with the slip direction. In face-centered cubic (FCC) metals, plastic deformation occurs primarily through the 12 $\{111\}\langle 110 \rangle$ systems, while body-centered cubic (BCC) metals use 24 systems composed by $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$.

When a single crystal is subjected to a macroscopic stress tensor σ , the resolved shear stress acting on each slip system α is obtained using the Schmid tensor M^α , defined by:

$$M^\alpha = b^\alpha \otimes n^\alpha \quad (2.12)$$

Where b^α is the slip direction and n^α the normal to the slip plane of system α . The resolved shear stress on slip system α is then:

$$\tau^\alpha = \sigma : \frac{1}{2}(M^\alpha + M^{\alpha,T}) = \sigma : M^\alpha \quad (2.13)$$

Because dislocation glide is a stress-driven mechanism, slip on a given slip plan can occur only when τ^α reaches the critical resolved shear stress τ_c . According to the generalized Schmid law, the yield criterion associated with activation of slip system α is therefore:

$$\begin{aligned} f^\alpha(\sigma_{ij}) &= \sigma : \frac{1}{2}(M^\alpha + M^{\alpha,T}) \\ &= \tau_c \end{aligned} \quad (2.14)$$

The associated flow rule gives the plastic strain-rate tensor produced by slip on system α as:

$$\dot{\epsilon}_p^\alpha = \dot{\lambda}^\alpha \frac{\partial f}{\partial \sigma} = \dot{\gamma}^\alpha \frac{1}{2}(M^\alpha + M^{\alpha,T}) \quad (2.15)$$

Where $\dot{\gamma}^\alpha$ is the dislocation slip rate on the slip system α .

The values of the different slip rates $\dot{\gamma}^\alpha$ for all active slip systems activated are obtained by minimizing the plastic work rate $\dot{W}$, which corresponds to minimizing the work rate associated with the internal friction from dislocation

glide (Taylor, 1938):

$$\begin{aligned}
 \dot{W} &= \sigma_{eq} \dot{\epsilon}_{eq,p} = \mathbf{s} : \dot{\epsilon}_p \\
 &= \sum_{\alpha} \mathbf{s} : \dot{\gamma}^{\alpha} \frac{1}{2} (\mathbf{M}^{\alpha} + \mathbf{M}^{\alpha,T}) \\
 &= \sum_{\alpha} \tau^{\alpha} \dot{\gamma}^{\alpha} \\
 &= \min \left(\sum_{\alpha} |\dot{\gamma}^{\alpha}| \tau_c \right)
 \end{aligned} \tag{2.16}$$

Where $\sigma_{eq} = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}}$ denotes the equivalent macroscopic stress and $\dot{\epsilon}_{eq,p} = \sqrt{\frac{2}{3} \dot{\epsilon}_p : \dot{\epsilon}_p}$ represents the equivalent plastic strain rate. Generally, activation of 5 independent slip systems is required to accommodate an arbitrary plastic strain state (Van Houtte et al., 2005).

For a given plastic strain-rate tensor $\dot{\epsilon}_p$ and the corresponding slip rates $\dot{\gamma}$, equation (2.16) defines a linear constraint representing a hyperplane in stress space that is tangent to the crystal yield locus. The complete single-crystal yield locus is therefore the envelope of all such hyperplanes corresponding to all stress states that permit dislocation glide along at least one slip system. If n hyperplanes intersect at a given stress state, this corresponds to a stress state activating n slip systems simultaneously (Van Houtte, 1987). The total plastic strain rate tensor of the crystal is thus:

$$\dot{\epsilon}_p = \sum_{\alpha} \dot{\gamma}^{\alpha} \frac{1}{2} (\mathbf{M}^{\alpha} + \mathbf{M}^{\alpha,T}) \tag{2.17}$$

The plastic work rate required to sustain a given $\dot{\epsilon}_p$ depends on the crystallographic orientation of the crystal. This orientation sensitivity is characterized by the Taylor factor M , defined as:

$$\begin{aligned}
 M &= \frac{\sigma_{eq}}{\tau_c} = \frac{\sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}}}{\tau_c} \\
 &= \frac{\sum_{\alpha} |\dot{\gamma}^{\alpha}|}{\dot{\epsilon}_{eq,p}} = \frac{\sum_{\alpha} |\dot{\gamma}^{\alpha}|}{\sqrt{\frac{2}{3} \dot{\epsilon}_p : \dot{\epsilon}_p}}
 \end{aligned} \tag{2.18}$$

A high Taylor factor reflects the need for larger slip activity and higher deviatoric stress to accommodate the imposed deformation, and therefore indicates a “harder” crystal orientation. The average Taylor factor of a polycrystal with an orientation distribution function $f(g)$ (ODF) over the polycrystal domain Ω is:

$$\langle M \rangle_{\Omega} = \oint M(g) f(g) dg \tag{2.19}$$

This quantity highlights the intrinsic link between crystallographic texture and macroscopic plastic anisotropy, since $\langle M \rangle_\Omega$ depends on the loading direction. For the specific case of plane strain compression, individual grains within a randomly oriented FCC polycrystal exhibit Taylor factors in the range $M \in [1.84, 4.22]$, while a random BCC aggregate typically fall within the range $M \in [1.78, 3.71]$ (Delannay, 2001).

When deforming a polycrystal, the flow stress increases with plastic strain, a phenomenon commonly referred to as strain hardening. This hardening arises from the multiplication of dislocations and the growing density of their interactions, which impede further dislocation motion. These interactions are generally divided into two categories: self-hardening and latent hardening (Asaro, 1983). Self-hardening results from interactions between dislocations belonging to the same slip system, whereas latent hardening originates from interactions between dislocations on different slip systems. With latent hardening, the activity of one slip system can increase the critical resolved shear stress (CRSS) of other systems, even if they remain inactive. Since the phenomena investigated here are not significantly influenced by strain hardening, we assume an identical critical resolved shear stress τ_c for all slip systems within the same grain, thereby accounting for both self- and latent hardening. This assumption results in an isotropic hardening behaviour at the polycrystal scale, while neglecting kinematic hardening contributions associated with the formation of dislocation substructures (dislocation pile-ups against grain boundaries and inclusions), which would otherwise induce directional hardening.

In addition to the Lankford coefficient used to characterize plastic behaviour, several other metrics are employed in this work. The first is the q -value, derived directly from the Lankford coefficient and defined as:

$$q = -\frac{\dot{\epsilon}_{yy,p}}{\dot{\epsilon}_{xx,p}} = \frac{R}{1 + R} \quad (2.20)$$

By definition, q ranges between 0 and 1. Since q and R are related through Equation (2.20), they provide equivalent information. However, the q -value often offers a more intuitive interpretation because it expresses the relative contraction in the y -direction for a given tensile strain in the x -direction. Plastic anisotropy can also be evaluated using the flow stress ratio defined as:

$$\frac{\sigma_{\text{yield}}(\psi)}{\sigma_{\text{yield}}(90^\circ)} \quad (2.21)$$

Here, $\sigma_{\text{yield}}(\psi)$ denotes the yield stress measured when the tensile axis is inclined by an angle ψ with respect to a reference direction, while $\sigma_{\text{yield}}(90^\circ)$

corresponds to the yield stress in the transverse (90°) direction. This ratio quantifies the dependence of the yield stress on the loading orientation for a fixed strain.

To characterize overall sheet anisotropy, the normal plastic anisotropy $\bar{R}$ and the planar plastic anisotropy ΔR are commonly defined as

$$\bar{R} = \frac{R0 + 2R45 + R90}{4} \quad \Delta R = \frac{R0 - 2R45 + R90}{2} \quad (2.22)$$

Where $R0$, $R45$ and $R90$ are the Lankford coefficients measured at 0° , 45° and 90° relative to the reference direction. The metric $\bar{R}$ indicates resistance to thickness reduction (higher values indicate better formability), while ΔR measures the tendency to form ears during deep drawing. An isotropic material satisfies $\Delta R = 0$.

2.3 Micro to macro modelling

It is well established that, although the macroscopic stress and strain fields in polycrystalline materials may appear uniform, the microscopic fields are highly heterogeneous due to the anisotropic mechanical response of individual grains. The local distribution of stress and strain among grains and even within a single grain is non-trivial as it must simultaneously satisfy stress equilibrium at grain boundaries and geometrical compatibility with adjacent grains. In this work, several crystal plasticity (CP) models are employed that satisfy these constraints either partially or fully, depending on the underlying modelling assumptions. These CP models provide a framework for predicting the macroscopic behaviour of polycrystalline aggregates while explicitly capturing the anisotropy of each grain. They also enable to investigate texture development.

The crystal plasticity models used in this work are grouped into two categories: mean-field crystal plasticity models and full-field crystal plasticity models.

2.3.1 Mean-field CP models

The first models presented are those classified as mean-field crystal plasticity models. We call them "mean-field" as they assume a homogeneous deformation within each grain of the deformed polycrystal. For this type of model, it has been shown that accounting for interactions with neighbouring grains can significantly influence the quality of predictions for both texture development and induced plastic anisotropy (Sidor, 2018). Accordingly, three different mean-field models, each incorporating varying levels of consideration for neighbouring grains, are presented in this section and employed throughout this work. A key advantage of these models is their ability to predict

macroscopic behaviour from microscopic material properties while requiring relatively low computational resources, in terms of both memory and CPU time.

2.3.1.1 Taylor FC

This model assumes that each grain of the polycrystal deforms according to a velocity gradient L_{gr} which is the same and equal to the macroscopic velocity gradient of the polycrystal L_{macro} (Taylor, 1938).

$$L_{gr} = L_{macro} \quad (2.23)$$

In this model, no misfit between individual grains is allowed due to the strict geometrical constraints imposed, as shown in Figure 2.9. Consequently, interactions with neighbouring grains are not considered. While the model accurately reproduces the macroscopic strain (verifying the deformation compatibility), the stress developing in each grain differs, due to the anisotropy and the heterogeneity of crystallographic orientations. As a result, stress equilibrium across grain boundaries is not satisfied (Hu et al., 2005).

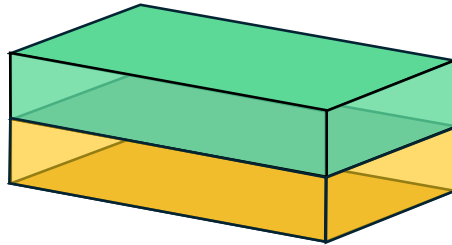


Figure 2.9: Illustration of two grains deforming under the Taylor full-constraint (FC) hypothesis. Each grain experiences the same velocity gradient as the macroscopic polycrystal.

In simulations, the macroscopic velocity gradient L_{macro} is prescribed to every grain and the stress and lattice rotation are calculated. The macroscopic stress is obtained by volume averaging over the polycrystal.

2.3.1.2 Taylor RC

The Taylor relaxed-constraint (RC) model provides a first compromise between the Taylor FC model, which assumes a uniform velocity gradient across all grains and thus enforces deformation compatibility between adjacent grains,

and the Sachs model, which assumes a uniform stress state and thereby satisfies stress equilibrium at grain boundaries. In Taylor RC, the deformation applied to each grain does not strictly correspond to the macroscopic velocity gradient as the shear strain parallel to the grain boundary are relaxed, whereas all remaining components must still correspond to L_{macro} . In this model, all grain boundaries are assumed to share the same orientation, perpendicular to the z -direction. This leads to the following expression for the grain velocity gradient:

$$L_{gr} = L_{macro} + \dot{\gamma}_{rlx}^{(1)} (\mathbf{p}^1 \otimes \mathbf{n}) + \dot{\gamma}_{rlx}^{(2)} (\mathbf{p}^2 \otimes \mathbf{n}) \quad (2.24)$$

Where $\mathbf{p}^1$ and $\mathbf{p}^2$ are two arbitrary orthogonal directions lying in the grain boundary plane and $\mathbf{n}$ denotes the normal to this boundary. The additional shear rates $\dot{\gamma}_{rlx}^{(1)}$ and $\dot{\gamma}_{rlx}^{(2)}$ are fictitious slip rates that allow relaxation of the corresponding velocity gradient components. Their values are determined by minimising the deformation energy, which is equivalent to enforcing the following conditions (Delannay et al., 2002):

$$\boldsymbol{\sigma} : (\mathbf{p}^1 \otimes \mathbf{n}) = \boldsymbol{\sigma} : (\mathbf{p}^2 \otimes \mathbf{n}) = 0 \quad (2.25)$$

These relations indicate that, in all grains, the shear stress components parallel to the grain boundary vanish. It thus ensures equilibrium of the shear stresses parallel to the grain boundary (which is not fulfilled with Taylor FC). However, Taylor RC model introduces strain incompatibilities between neighbouring grains, since the amount of relaxation generally differs from one grain to another, as shown in Figure 2.10. Interactions with neighbouring grains remain very much simplified, as the energy minimisation procedure is carried out independently for each grain (Van Houtte et al., 2005). Note that, in this work, this model is referred to as Taylor RC, although it is also known in the literature as the pancake model (Van Houtte, 1982).

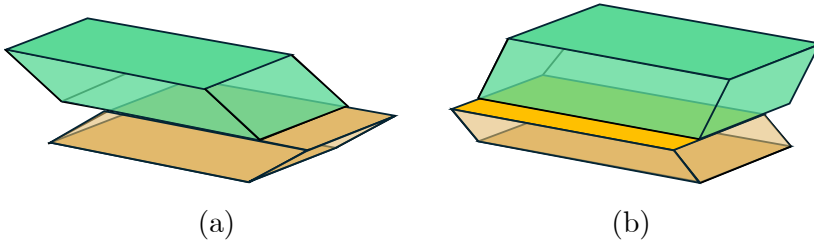


Figure 2.10: Illustration of two grains deforming under the Taylor relaxed-constraint (RC) model. Shear components parallel to the grain boundary are relaxed independently in each grain, ensuring continuity of shear stresses along boundaries while allowing strain incompatibility between neighbouring grains.

2.3.1.3 (A)LAMEL

Unlike the two previously presented models, the ALAMEL model accounts for the short-range interactions by treating each pair of adjacent grains with a distinct grain-boundary orientation. Rather than treating grains independently, the model evaluates the coupled deformation of grain pairs. Each pair of adjacent grains (Grain 1 and Grain 2) is assumed to deform jointly such that their average velocity gradient equals the macroscopic velocity gradient ($(\mathbf{L}_{gr1} + \mathbf{L}_{gr2})/2 = \mathbf{L}_{macro}$) while allowing relaxation through equal and opposite shear components parallel to the grain boundary, as illustrated in Figure 2.11. The constitutive expressions for the two interacting grains can therefore be written as:

$$\begin{aligned} \mathbf{L}_{gr1} &= \mathbf{L}_{macro} + \dot{\gamma}_{rlx}^{(1)} (\mathbf{p}^1 \otimes \mathbf{n}) + \dot{\gamma}_{rlx}^{(2)} (\mathbf{p}^2 \otimes \mathbf{n}) \\ \mathbf{L}_{gr2} &= \mathbf{L}_{macro} - \dot{\gamma}_{rlx}^{(1)} (\mathbf{p}^1 \otimes \mathbf{n}) - \dot{\gamma}_{rlx}^{(2)} (\mathbf{p}^2 \otimes \mathbf{n}) \end{aligned} \quad (2.26)$$

where $\mathbf{p}^1$ and $\mathbf{p}^2$ are two orthonormal vectors lying in the grain-boundary plane, and $\mathbf{n}$ denotes the corresponding grain boundary normal. The relaxation shear rates $\dot{\gamma}_{rlx}^{(1)}$ and $\dot{\gamma}_{rlx}^{(2)}$ are chosen to minimise the deformation energy, which is equivalent to enforcing the following conditions on the Cauchy stresses of the two grains (Delannay et al., 2008):

$$(\boldsymbol{\sigma}_{gr1} - \boldsymbol{\sigma}_{gr2}) : (\mathbf{p}^1 \otimes \mathbf{n}) = (\boldsymbol{\sigma}_{gr1} - \boldsymbol{\sigma}_{gr2}) : (\mathbf{p}^2 \otimes \mathbf{n}) = 0 \quad (2.27)$$

These conditions ensure that both grains experience identical shear-stress components parallel to the grain boundary. Because the deformation energy is minimised jointly for the two interacting grains, short-range grain interactions are incorporated which is not the case for the Taylor-type models. Indeed, with ALAMEL, the deformation of a given grain is influenced by the crystallographic orientation of its neighbouring grain. Consequently, Equations (2.26) and (2.27) enforce both deformation compatibility across the grain boundary and equilibrium of the corresponding shear stresses. The ALAMEL model has shown to provide superior predictions of both crystallographic texture and plastic anisotropy when compared with the other mean-field models discussed previously (Van Houtte et al., 1999, 2002; Zhang et al., 2014, 2015; Manik et al., 2021).

In this model, the grain-boundary orientation $\mathbf{n}$ is assigned randomly for a pair of grains and is determined from the average grain shape in the studied microstructure. The grain shape is represented by an ellipsoid with principal diameters a , b , and c , such that $a = b = c = 1$ for an equiaxed grain. Therefore, for each grain, the initial grain-boundary normal is obtained from a random vector (x_1, x_2, x_3) through:

$$\mathbf{n}_{init} = \left(\frac{x_1}{a}, \frac{x_2}{b}, \frac{x_3}{c} \right) / \sqrt{\left(\frac{x_1}{a} \right)^2 + \left(\frac{x_2}{b} \right)^2 + \left(\frac{x_3}{c} \right)^2} \quad (2.28)$$

This normal is updated at each increment of time according to the macroscopic deformation using Nanson's relation: $\mathbf{n} = (\mathbf{F}^{-1})^T : \mathbf{n}_{init}$.

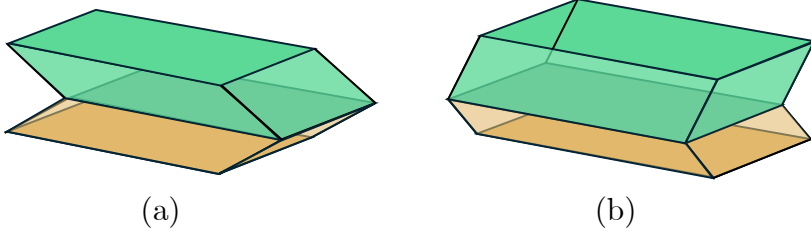


Figure 2.11: Illustration of two interacting grains under the ALAMEL model. Short-range interactions are accounted for by enforcing continuity of shear stress components parallel to the grain boundary and strain comparability as the pair of grain experiences the same velocity gradient as the macroscopic velocity gradient.

Note that the well-known CP model named LAMEL model is similar to ALAMEL, but all the grain boundaries are assumed to lie in the RD–TD plane (Van Houtte et al., 2002).

In certain simulations, some components of the macroscopic velocity gradient are not prescribed, while the corresponding components of the stress tensor are constrained. A typical example is a uniaxial tensile test, where the velocity gradient component along the loading direction is prescribed, whereas the components in the perpendicular directions are unknown. However, in these directions, the macroscopic stress must remain null. Another example is the elastic springback after plastic deformation where none of the velocity gradient components are known, yet the resulting macroscopic stress must vanish. For simulations that are partially (tensile test) or fully (elastic recovery) stress-controlled, an additional Newton–Raphson iterative loop is used at each time step to correct the macroscopic velocity gradient components which are not directly prescribed, ensuring the macroscopic stress constraints are satisfied. This correction procedure requires the derivation of the macroscopic consistent tangent operator $\frac{\partial \Delta \sigma_{macro}}{\partial \Delta D_{macro}}$. Further details concerning the approach to treat the stress-controlled simulations can be found in Delannay et al. (2002). The same procedure is applicable for all other mean-field models considered in this work.

2.3.1.4 Other mean-field models

Several other mean-field crystal plasticity models, widely used in the literature, are relevant to the study of polycrystalline deformation and texture evolution but were not used in this work. Nevertheless, a brief overview of these models is provided below.

Visco-plastic self-consistent (VPSC) model is based on the Eshelby inclusion problem (Lebensohn and Tomé, 1993). Here, each grain is treated as an inclusion embedded within a homogeneous equivalent medium whose properties are determined from the overall grain aggregate. The model calculates the interaction between the inclusion and its surrounding medium, allowing the prediction of heterogeneous plastic deformation within individual grains. Thus, long-range interactions (reflecting the influence of the embedding medium on the grain) are accounted for through the homogeneous medium in VPSC model.

The Grain Interaction (GIA) model can be considered as an extension of the LAMEL model to an eight-grain assembly (Crumbach et al., 2001). It considers an eight-grain aggregate, which is subdivided into four two-grain stacks. Each stack deforms to satisfy the imposed macroscopic deformation while allowing the same relaxation as in the LAMEL model. Although the individual stacks can reproduce the macroscopic deformation, mismatches between stacks may arise. To address this, a penalty function based on the density of geometrically necessary dislocations (GNDs) is introduced to enforce inter-grain compatibility.

2.3.2 Full-field model - CPFEM

Full-field models are considered as the most comprehensive approaches for crystal plasticity simulations. In addition to capturing the macroscopic mechanical response and evolution of texture, full-field models can resolve the micromechanical fields while accounting for the exact microstructural geometry. These methods ensure both strain compatibility and stress equilibrium at every crystalline interface (Roters et al., 2010). Because full-field approaches incorporate both short-range and long-range interactions in the mechanical response of each grain, they generally provide superior accuracy, but this comes with a significantly higher computational cost.

Two models are commonly categorized as full-field approaches: Crystal Plasticity Finite Element Method (CPFEM) (Peirce et al., 1982) and Crystal Plasticity Fast Fourier Transform (CP-FFT) method (Lebensohn, 2001). The latter will not be detailed here as only CPFEM was used in this work.

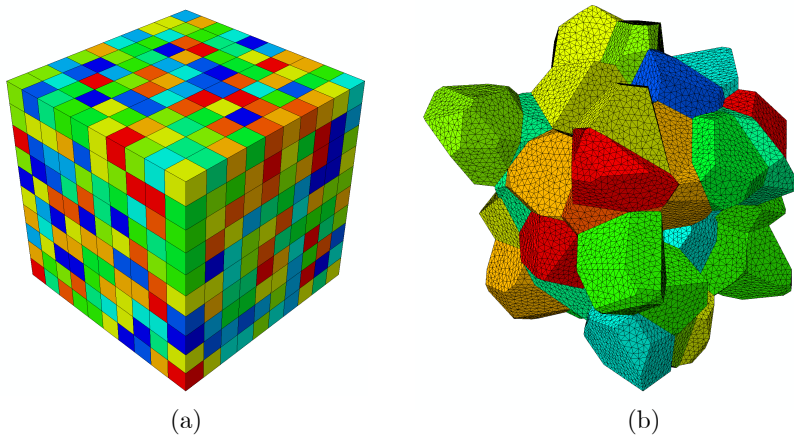


Figure 2.12: Examples of microstructural geometries used in CPFEM simulations: (a) idealized uniform brick-shaped grains with one orientation per element and (b) more realistic geometry generated via Voronoi tessellation, where multiple finite elements compose a single grain.

In CPFEM, the geometry of microstructure is discretized using finite elements and a single crystallographic orientation is assigned to all integration points belonging to the same grain. As shown in Figure 2.12, "realistic" microstructural geometries and their corresponding meshes can be generated using Voronoi tessellations from a set of seeds distributed uniformly across a domain, in gmsh (Geuzaine and Remacle, 2009), whereas more idealized and structured microstructures, meshed with uniform brick-shaped elements, are produced using an homemade code (Melchior, 2009). Periodic boundary conditions (PBC) are generally applied so that peripheral grains behave as if they were embedded in the bulk. Mathematical details concerning PBC are presented in Appendix F.

Crystal plasticity constitutive laws are implemented in a user subroutine (UMAT) in Abaqus. The fully implicit solver of Abaqus makes use of this UMAT to calculate, at each time increment, the Cauchy stress tensor σ , solution-dependent state variables and the consistent tangent operator $\frac{\partial \Delta \sigma}{\partial \Delta D}$. This tangent operator is required to correctly linearize the user-defined constitutive equations. A detailed derivation of this operator is provided in (Delannay et al., 2006). Abaqus then computes $\Delta \epsilon$ and $\Delta R_{r,b}$ for the next time increment.

2.4 Derivation of the equations governing crystal plasticity theory

Before concluding the chapter with the presentation of the detailed objectives addressed in this thesis, this section provides the derivation of the governing equations of crystal plasticity. These derivations are essential for understanding the formulation and numerical implementation of the various crystal plasticity (CP) models examined in this work. Details concerning the numerical implementation are also discussed at the end of the section.

The UMAT used in Abaqus, as well as the Fortran files containing the mean-field models, were not implemented as part of this thesis.

2.4.1 Mathematical framework for finite deformation

Plastic deformation processes, such as rolling, can induce substantial changes in the geometry of a material body relative to its reference configuration. To accurately describe and track the evolution of deformation throughout the entire history, a rigorous and well-posed mathematical framework is necessary. Let the relative position of a material point with respect to a neighbouring point in the reference configuration be represented by the vector $d\mathbf{X}$. The magnitude of this vector is infinitesimally small. When the body undergoes deformation, this vector is modified by an incremental displacement $d\mathbf{u}$, such that the corresponding vector in the current configuration, $d\mathbf{x}$, satisfies:

$$d\mathbf{x} = d\mathbf{X} + d\mathbf{u} \quad (2.29)$$

The deformation gradient $\mathbf{F}$ establishes the relationship between the differential vectors before and after deformation, and is defined as:

$$d\mathbf{x} = \left(\frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right) d\mathbf{X} = \left(\mathbf{I} + \frac{\partial \mathbf{u}}{\partial \mathbf{X}} \right) d\mathbf{X} = \mathbf{F} d\mathbf{X} \quad (2.30)$$

Here, $\mathbf{I}$ is the second-order identity tensor. Since the deformation gradient is invertible (the eigenvalues are strictly positive), it can be decomposed into a orthogonal rotation tensor $\mathbf{R}$ and a symmetric stretch tensor, expressed either as the right stretch $\mathbf{U}$ or the left stretch $\mathbf{V}$, such that:

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R} \quad (2.31)$$

The corresponding Lagrangian strain tensor E is defined as:

$$\begin{aligned}
 E &= \frac{1}{2} \left(F^T F - I \right) \\
 &= \frac{1}{2} \left((RU)^T (RU) - I \right) \\
 &= \frac{1}{2} \left(U^T R^T RU - I \right) \\
 &= \frac{1}{2} \left(U^T U - I \right)
 \end{aligned} \tag{2.32}$$

Plastic deformation is inherently path-dependent: several metal sheets following different deformation histories but reaching the same final states will have distinct internal states variables (stress, plastic strain, ...). Consequently, plastic constitutive models are formulated in rate form to account for this history dependence (Melchior, 2009). The velocity gradient tensor L represents the spatial gradient of the material velocity and is defined as:

$$L = \dot{F} F^{-1} \tag{2.33}$$

This tensor can be decomposed into a symmetric part, corresponding to the rate of deformation tensor D , and an antisymmetric part, corresponding to the spin tensor W , as follows:

$$D = \frac{1}{2} (L + L^T) \quad W = \frac{1}{2} (L - L^T) \tag{2.34}$$

2.4.2 Governing equations of crystal plasticity

The theoretical framework presented in this section applies exclusively to metals in which plastic deformation occurs solely through dislocation slip. Mechanisms such as mechanical twinning and transformation-induced plasticity are not considered in the present formulation. The following equations are based on the crystal plasticity framework developed in (Delannay et al., 2006). Since the early developments of constitutive equations for single-crystal plasticity, the deformation gradient has been decomposed into two distinct contributions (Hill and Rice, 1972; Asaro, 1983; Kalidindi et al., 1992):

$$F = F^* F_p = R^* U_{el} F_p \tag{2.35}$$

Here, F_p represents the plastic part of the deformation gradient, which maps the initial configuration to an intermediate configuration corresponding to the deformation resulting from the dislocation slip only. This contribution is irreversible and permanent, while preserving the lattice geometry, as shown in Figure 2.13 (Roters et al., 2010). The tensor F^* then maps the intermediate

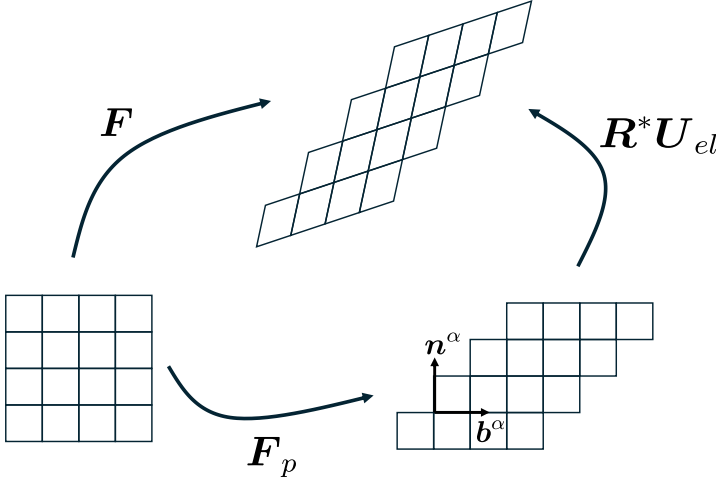


Figure 2.13: Multiplicative decomposition of the deformation gradient F into a plastic contribution F_p , which produces a fictitious intermediate configuration, followed by the elastic stretch tensor U_{el} and the lattice rotation tensor R^* , enabling to obtain the total deformation.

configuration to the final deformed configuration. It is composed by a symmetric elastic stretch tensor U_{el} , accounting for the reversible lattice distortion, and a rotation tensor R^* which represents the lattice rotation resulting from slip activity on the activated slip systems. Based on this decomposition, the velocity gradient can be expressed as:

$$\begin{aligned}
 L &= \dot{F}F^{-1} = (\dot{R}^* \dot{U}_{el} F_p) (R^* U_{el} F_p)^{-1} \\
 &= (\dot{R}^* U_{el} F_p + R^* \dot{U}_{el} F_p + R^* U_{el} \dot{F}_p) (F_p^{-1} U_{el}^{-1} R^{*-1}) \\
 &= (\dot{R}^* U_{el} F_p + R^* \dot{U}_{el} F_p + R^* U_{el} \dot{F}_p) (F_p^{-1} U_{el}^{-1} R^{*T}) \\
 &= \dot{R}^* U_{el} F_p F_p^{-1} U_{el}^{-1} R^{*T} + R^* \dot{U}_{el} F_p F_p^{-1} U_{el}^{-1} R^{*T} + R^* U_{el} \dot{F}_p F_p^{-1} U_{el}^{-1} R^{*T} \\
 &= \dot{R}^* R^{*T} + R^* \dot{U}_{el} U_{el}^{-1} R^{*T} + R^* U_{el} \dot{F}_p F_p^{-1} U_{el}^{-1} R^{*T} \\
 &= \boxed{\dot{R}^* R^{*T} + R^* \dot{U}_{el} U_{el}^{-1} R^{*T} + R^* U_{el} L_p U_{el}^{-1} R^{*T}}
 \end{aligned} \tag{2.36}$$

Here, the plastic velocity gradient L_p results from the cumulative effect of dislocation glide on all active slip systems:

$$L_p = \dot{F}_p F_p^{-1} = \sum_{\alpha} (b^{\alpha} \otimes n^{\alpha}) \dot{\gamma}^{\alpha} = \sum_{\alpha} M^{\alpha} \dot{\gamma}^{\alpha} \tag{2.37}$$

Here, b^{α} and n^{α} denote the slip direction and the slip-plane normal of system α , respectively, and the dyadic product of these two vectors gives the Schmid

tensor $\mathbf{M}^\alpha$. The term $\dot{\gamma}^\alpha$ represents the shear rate on the corresponding slip system.

Based on Equation (2.32), the elastic Green strain tensor is defined as:

$$\mathbf{E} = \frac{1}{2} \left(\mathbf{U}_{el}^T \mathbf{U}_{el} - \mathbf{I} \right) \quad (2.38)$$

The stress tensor being work-conjugated to $\mathbf{E}$ is the second Piola–Kirchhoff stress tensor $\mathbf{T}$, which is defined in the intermediate configuration. It is related to the Cauchy stress tensor $\boldsymbol{\sigma}$, defined in the current configuration, by

$$\begin{aligned} \mathbf{T} &= \det(\mathbf{F}_{el}) \mathbf{F}^{-1} \boldsymbol{\sigma} \mathbf{F}^{-T} \\ &= \det(\mathbf{R}_{el}^*) \det(\mathbf{U}_{el}) (\mathbf{R}_{el}^* \mathbf{U}_{el})^{-1} \boldsymbol{\sigma} (\mathbf{R}_{el}^* \mathbf{U}_{el})^{-T} \\ &= \det(\mathbf{U}_{el}) \mathbf{U}_{el}^{-1} \mathbf{R}_{el}^{*T} \boldsymbol{\sigma} \mathbf{R}_{el}^* \mathbf{U}_{el}^{-1} \end{aligned} \quad (2.39)$$

The linear coupling between the elastic stress tensor $\mathbf{T}$ and elastic strain tensor $\mathbf{E}$ is made through the fourth-order tensor containing the elastic stiffness constant $\mathbf{C}$:

$$\mathbf{T} = \mathbf{C} : \mathbf{E} \quad (2.40)$$

As mentioned in Section 2.1, dislocation glide is a stress-driven mechanism. Slip on a system α occurs when the applied shear stress τ^α reaches the corresponding critical resolved shear stress of the corresponding slip plan τ_c^α :

$$|\tau^\alpha| \leq \tau_c^\alpha \quad (2.41)$$

The shear stress τ^α can be obtained by projecting the second Piola–Kirchhoff stress tensor onto the slip system using the Schmid tensor:

$$\tau^\alpha = \mathbf{T} : \mathbf{M}^\alpha \quad (2.42)$$

The sign of τ^α determines the direction of dislocation motion on the corresponding slip system.

2.4.3 Hypotheses and phenomenological constitutive models

During metal forming, the prescribed deformation can be very large, leading to plastic strains that are much greater than the elastic ones. Consequently, it is reasonable to assume that the elastic strains are infinitesimally small. Under this assumption, the elastic stretch tensor $\mathbf{U}_{el}$ can be approximated as $\mathbf{U}_{el} = \mathbf{I} + \boldsymbol{\varepsilon}_{el}$ where $\boldsymbol{\varepsilon}_{el}$ is a symmetric second-order tensor satisfying $\|\boldsymbol{\varepsilon}_{el}\|^2 \ll 1$. From this definition, the following first-order approximations gives:

$$(\mathbf{U}_{el})^{-1} = \mathbf{I} - \boldsymbol{\varepsilon}_{el} \quad (2.43)$$

$$\det(\mathbf{U}_{el}) = 1 + \text{tr}(\boldsymbol{\varepsilon}_{el}) \quad (2.44)$$

Where $\text{tr}(\cdot)$ denotes the trace operator. Substituting these approximations into equation (2.36) leads to the simplified expression of the velocity gradient $\mathbf{L}$:

$$\begin{aligned} \mathbf{L} &= \dot{\mathbf{R}}^* \mathbf{R}^{*T} + \mathbf{R}^* \dot{\mathbf{U}}_{el} \mathbf{U}_{el}^{-1} \mathbf{R}^{*T} + \mathbf{R}^* \mathbf{U}_{el} \mathbf{L}_p \mathbf{U}_{el}^{-1} \mathbf{R}^{*T} \\ &= \dot{\mathbf{R}}^* \mathbf{R}^{*T} + \mathbf{R}^* \dot{\boldsymbol{\varepsilon}}_{el} (\mathbf{I} - \boldsymbol{\varepsilon}_{el}) \mathbf{R}^{*T} + \mathbf{R}^* (\mathbf{I} + \boldsymbol{\varepsilon}_{el}) \mathbf{L}_p (\mathbf{I} - \boldsymbol{\varepsilon}_{el}) \mathbf{R}^{*T} \\ &= \dot{\mathbf{R}}^* \mathbf{R}^{*T} + \mathbf{R}^* \dot{\boldsymbol{\varepsilon}}_{el} \mathbf{R}^{*T} + \mathbf{R}^* \mathbf{L}_p \mathbf{R}^{*T} \\ &= \dot{\mathbf{R}}^* \mathbf{R}^{*T} + \mathbf{R}^* (\dot{\boldsymbol{\varepsilon}}_{el} + \mathbf{L}_p) \mathbf{R}^{*T} \end{aligned} \quad (2.45)$$

Similarly, the expression of the second Piola–Kirchhoff stress tensor $\mathbf{T}$, in equation (2.39) can be reduced to:

$$\begin{aligned} \mathbf{T} &= \det(\mathbf{U}_{el}) \mathbf{U}_{el}^{-1} \mathbf{R}^{*T} \boldsymbol{\sigma} \mathbf{R}^* \mathbf{U}_{el}^{-1} \\ &= (1 + \text{tr}(\boldsymbol{\varepsilon}_{el})) (\mathbf{I} - \boldsymbol{\varepsilon}_{el}) \mathbf{R}^{*T} \boldsymbol{\sigma} \mathbf{R}^* (\mathbf{I} - \boldsymbol{\varepsilon}_{el}) \\ &= \mathbf{R}^{*T} \boldsymbol{\sigma} \mathbf{R}^* \end{aligned} \quad (2.46)$$

The Green–Lagrange strain tensor $\mathbf{E}$ can also be simplified under the same assumption:

$$\begin{aligned} \mathbf{E} &= \frac{1}{2} \left(\mathbf{U}_{el}^T \mathbf{U}_{el} - \mathbf{I} \right) \\ &= \frac{1}{2} \left((\mathbf{I} + \boldsymbol{\varepsilon}_{el})^T (\mathbf{I} + \boldsymbol{\varepsilon}_{el}) - \mathbf{I} \right) \\ &= \frac{1}{2} \left((\mathbf{I} + \boldsymbol{\varepsilon}_{el}) (\mathbf{I} + \boldsymbol{\varepsilon}_{el}) - \mathbf{I} \right) \\ &= \frac{1}{2} (\mathbf{I} + \boldsymbol{\varepsilon}_{el} + \boldsymbol{\varepsilon}_{el} + \boldsymbol{\varepsilon}_{el} \boldsymbol{\varepsilon}_{el} - \mathbf{I}) \\ &= \boldsymbol{\varepsilon}_{el} \end{aligned} \quad (2.47)$$

By combining the above relations, the constitutive equation of linear elasticity is obtained as:

$$\mathbf{T} = \mathbf{R}^{*T} \boldsymbol{\sigma} \mathbf{R}^* = \mathbf{C} : \boldsymbol{\varepsilon}_{el} \quad (2.48)$$

Historically, the activation of slip systems and the corresponding shear strain rates $\dot{\gamma}^\alpha$ have been determined using an energetic minimization principle. This principle seeks to minimize the total work rate associated with the internal friction from dislocation glide (Taylor, 1938). This approach is rate insensitive and expresses as :

$$\min \left(\sum_{\alpha} \tau_c |\dot{\gamma}_\alpha| \right) \quad (2.49)$$

Where the critical resolved shear stress is assumed uniform across all slip systems ($\tau_c^\alpha = \tau_c$). However, this assumption leads to a non-unique solution,

known as the *Taylor ambiguity*, since multiple combinations of 5 slip systems can produce the desired deformation and achieve the same minimum energy state (Mánik and Holmedal, 2014). To circumvent this limitation, a viscoplastic exponential law is adopted to relate the slip rate $\dot{\gamma}^\alpha$ to the resolved shear stress τ^α acting on slip system α (Hutchinson, 1977). The law corresponds to:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{\tau_c^\alpha} \right|^{1/m} \text{sign}(\tau_c^\alpha) \quad (2.50)$$

Where m is the strain rate sensitivity exponent and $\dot{\gamma}_0$ is the reference shear rate. The use of this formulation implies that all slip systems exhibit nonzero shear rates, in contrast to the rate-insensitive theory, which typically predicts activity on only five independent slip systems (Taylor, 1938; Bishop and Hill, 1951b,a). Nevertheless, the slip systems associated with the highest shear rates correspond to those that would be activated using the rate-insensitive theory (Van Houtte et al., 2005).

The increase in the critical resolved shear stress during plastic deformation is attributed to dislocation interactions, which hinder dislocation motion as deformation proceeds. To model this hardening behavior, a Swift-type isotropic hardening law is employed (Raveendra et al., 2011):

$$\tau_c = \tau_{c0} \left(1 + \frac{\Gamma_{tot}}{\Gamma_0} \right)^n \quad (2.51)$$

$$\Gamma_{tot} = \int_0^t \sum_\alpha |\dot{\gamma}^\alpha| dt \quad (2.52)$$

Where τ_{c0} , Γ_0 and n are material properties. This expression establishes the coupling between the slip rate $\dot{\gamma}^\alpha$ and the evolving critical resolved shear stress $\tau_{c,\alpha}$. In this work, the same resolved shear stress is assumed for all slip systems

2.4.4 Implicit time-integration of constitutive equations and implementation details

The crystal plasticity theory and the associated constitutive models are reformulated into an implicit time-integration scheme suitable for numerical implementation. Additional details regarding the derivation of these equations can be found in Delannay et al. (2006).

Taking the symmetric part of the velocity gradient increment ΔL over a time step Δt in Equation (2.45) gives :

$$\Delta D = \mathbf{R}^*|_{t+\Delta t} \left[\dot{\epsilon}_{el} + \frac{1}{2} \left(\mathbf{L}_p + \mathbf{L}_p^T \right) \right] \mathbf{R}^{*T}|_{t+\Delta t} \Delta t \quad (2.53)$$

Isolating the increment of elastic strain $\dot{\epsilon}_{el}\Delta t$ and substituting Equation (2.37), the elastic strain increment becomes a function of the slip increments $\Delta\gamma$ the total rate of deformation tensor ΔD as:

$$\dot{\epsilon}_{el}\Delta t = R^{*T}|_{t+\Delta t}\Delta DR^*|_{t+\Delta t} - \sum_{\alpha} \left[\frac{1}{2} \left(M^{\alpha} + M^{\alpha,T} \right) \Delta\gamma^{\alpha} \right] \quad (2.54)$$

Using the linear elastic law expressed in the Equation (2.40), the increment of the second Piola–Kirchhoff stress tensor T follows as:

$$T|_{t+\Delta t} = T|_t + C \left(R^{*T}|_{t+\Delta t}\Delta DR^*|_{t+\Delta t} - \frac{1}{2} \sum_{\alpha} \left(M^{\alpha} + M^{\alpha,T} \right) \Delta\gamma^{\alpha} \right) \quad (2.55)$$

Since the lattice rotation increments are very small over a single time step, the $R^{*T}|_{t+\Delta t}\Delta DR^*|_{t+\Delta t}$ is expanded using the lattice spin tensor $\Omega^* = \dot{R}^*|_{t+\Delta t}R^{*T}|_{t+\Delta t}$, which is more convenient from a numerical viewpoint, as:

$$\begin{aligned} R^{*T}|_{t+\Delta t}\Delta DR^*|_{t+\Delta t} &= R^{*T}|_t\Delta DR^*|_t + \left(\dot{R}^{*T}|_{t+\Delta t}\Delta DR^*|_{t+\Delta t} + R^{*T}|_{t+\Delta t}\Delta D\dot{R}^*|_{t+\Delta t} \right) \Delta t \\ &= R^{*T}|_t\Delta DR^*|_t + \left(\dot{R}^{*T}|_{t+\Delta t}R^*|_{t+\Delta t}\Delta D + \Delta DR^*|_{t+\Delta t}\dot{R}^*|_{t+\Delta t} \right) \Delta t \\ &= R^{*T}|_t\Delta DR^*|_t + (-\Omega^*\Delta D + \Delta D\Omega^*) \Delta t \\ &= R^{*T}|_t\Delta DR^*|_t + (\Delta D\Omega^*|_{t+\Delta t} - \Omega^*|_{t+\Delta t}\Delta D) \Delta t \end{aligned} \quad (2.56)$$

Substituting this expression into Equation (2.55) gives:

$$T|_{t+\Delta t} = T|_t + C \left(R^{*T}|_t\Delta DR^*|_t + (\Delta D\Omega^*|_{t+\Delta t} - \Omega^*|_{t+\Delta t}\Delta D) \Delta t - \frac{1}{2} \sum_{\alpha} \left(M^{\alpha} + M^{\alpha,T} \right) \Delta\gamma^{\alpha} \right) \quad (2.57)$$

Equation (2.57) shows that T depends on the slip increment $\Delta\gamma$. Conversely, the slip increments themselves depend on the stress. Indeed, combining Equation (2.50) with (2.42) gives:

$$\Delta\gamma^{\alpha} = \dot{\gamma}^{\alpha}\Delta t = \dot{\gamma}_0 \left| \frac{M^{\alpha} : T|_{t+\Delta t}}{\tau_c^{\alpha}} \right|^{1/m} \text{sign}(\tau_c^{\alpha}) \quad (2.58)$$

which confirms the mutual dependence between $\Delta\gamma$ and $T|_{t+\Delta t}$. This stress tensor also depends on the critical resolved shear stress τ_c , which must be updated after each slip increment. Using the hardening law, the total accumulated slip and the CRSS evolve as:

$$\tau_c|_{t+\Delta t} = \tau_{c0} \left(1 + \frac{\Gamma_{tot}|_{t+\Delta t}}{\Gamma_0} \right)^n \quad (2.59)$$

$$\Gamma_{tot}|_{t+\Delta t} = \Gamma_{tot}|_t + \sum_{\alpha} |\Delta\gamma^{\alpha}| \quad (2.60)$$

The system (2.57), (2.58), (2.59), (2.60) is solved using a two-level Newton-Raphson scheme. The outer Newton-Raphson iteration determines the best estimates of the six independent components of the second Piola-Kirchhoff stress tensor, $T|_{t+\Delta t}$, while holding the critical resolved shear stresses τ_c^α fixed. Within each outer iteration, an inner Newton-Raphson loop is employed to compute the best estimates of the slip increments $\Delta\gamma^\alpha$ on all active slip systems, based on the current estimate of the stress state. Once the convergence criteria for both loops are satisfied, the updated values of $T|_{t+\Delta t}$, $\Delta\gamma^\alpha$ and τ_c^α are obtained.

The rotation matrix defining the lattice rotation R^* is calculated by considering the antisymmetric part of Equation (2.45), which gives the lattice spin, noted Ω^* , as

$$\dot{R}^*|_{t+\Delta t} R^{*T}|_{t+\Delta t} = W|_{t+\Delta t} - R^*|_{t+\Delta t} W_p|_{t+\Delta t} R^{*T}|_{t+\Delta t} = \Omega^*|_{t+\Delta t} \quad (2.61)$$

Where W is the total spin tensor and W_p is the plastic spin tensor obtained from the antisymmetric part of the velocity gradient L_p . This relation expresses the kinematic constraint associated with texture evolution as illustrated in Figure 2.5.

Quaternion related to the lattice rotation q^* can be derived using the exponential map (Simo and Hughes, 1998) as:

$$\begin{aligned} q_0^* &= \cos(\omega) & q_1^* &= \frac{1}{2} \frac{\Omega_{23}^*}{(\|\Omega\|/2)} \sin(\omega) \\ q_2^* &= \frac{1}{2} \frac{\Omega_{13}^*}{(\|\Omega\|/2)} \sin(\omega) & q_3^* &= \frac{1}{2} \frac{\Omega_{12}^*}{(\|\Omega\|/2)} \sin(\omega) \end{aligned} \quad (2.62)$$

with $\omega = \frac{\|\Omega^*\| \Delta t}{2}$. We can then obtain from the quaternion the corresponding rotation matrix R^* using Appendix D. If, during the simulation, the lattice spin Ω^* reaches 0 and remains 0 thereafter, it indicates that a stable crystallographic orientation has been reached, as illustrated in Figure 2.6.

Finally, the updated Cauchy stress is obtained from:

$$\sigma|_{t+\Delta t} = R^*|_{t+\Delta t} T|_{t+\Delta t} R^{*T}|_{t+\Delta t} \quad (2.63)$$

In the iterative system (2.57), (2.58), (2.60), the rotation matrix $R^*|_{t+\Delta t}$ is not known a priori. An initial estimate is obtained from $R^*|_{t+\Delta t} \approx \Delta R R^*|_t$ which can be used to make all the calculations and obtain a new approximation of $R^*|_{t+\Delta t}$. This updated rotation is then reintroduced into the constitutive equations to recompute $T|_{t+\Delta t}$, $\Delta\gamma^\alpha$ and τ_c^α . Further details regarding this approximation are provided in Delannay et al. (2006).

These formulations of the crystal plasticity constitutive relations, combined with the different modelling hypotheses underlying the various CP

C_{11}	C_{12}	C_{44}	m	$\dot{\gamma}_0$	Γ_0	n	τ_{c0}
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Table 2.2: List of microscopic material parameters used as input for the crystal plasticity models. These parameters are fitted to experimental data to accurately reproduce the macroscopic mechanical response.

models, were implemented numerically in a Fortran code for the mean-field models and in a UMAT for the CPFEM. The codes take as input the crystallographic orientations of all grains composing the polycrystal. In addition, microscopic elastic and plastic material parameters must be prescribed. These parameters are listed in Table 2.2. Due to the cubic symmetry of FCC and BCC crystals, only three independent constants are required to describe the elastic stiffness matrix. All material parameters must be calibrated against experimental data to accurately reproduce the macroscopic behaviour.

For clarity, only the algorithm underlying the CPFEM implementation (Algorithm 1) is presented in this section. The implementations of the Taylor FC, Taylor RC, and ALAMEL models are provided in Appendix E.

Algorithm 1 CPFEM

Input: $L|_{t+\Delta t}$

Output: $R^*|_{t+\Delta t}$, $\sigma|_{t+\Delta t}$, $\frac{\partial \Delta \sigma}{\partial \Delta D}$, $\sigma|_{t+\Delta t}$

for element do

for integration point do

$T|_{t+\Delta t} = T|_t$

$\tau_c|_{t+\Delta t} = \tau_c|_t$

while $\|T^i - T^{i+1}\| > tol$ **do**

▷ N-R scheme

while $\|\tau_c^j - \tau_c^{j+1}\| > tol$ **do**

▷ N-R scheme

$T^i \rightarrow \Delta \gamma^\alpha$

▷ Equations (2.58), (2.59), (2.60)

$\Delta \gamma^\alpha \rightarrow \tau_c^{j+1}$

▷ Equations (2.59), (2.60)

end while

$\dot{\gamma}^{\alpha,i} \rightarrow L_p^i$

▷ Equation (2.37)

$L, L_p^i \rightarrow \Omega^{*,i}, R^{*,i}$

▷ Equation (2.62)

$L, \Omega^{*,i}, \dot{\gamma}^{\alpha,i} \rightarrow T^{i+1}$

▷ Equations (2.58), (2.57)

end while

$T|_{t+\Delta t}, R^*|_{t+\Delta t} \rightarrow \sigma|_{t+\Delta t}$

▷ Equation (2.63)

$T|_{t+\Delta t}, R^*|_{t+\Delta t}, L \rightarrow \frac{\partial \Delta \sigma}{\partial \Delta D}$

end for

end for

2.5 Objectives of the thesis

This chapter highlights the strong interplay between plastic deformation and crystallographic texture. Specifically, plastic deformation modifies the texture, while the existing texture influences the plastic anisotropy response in metallic alloys. This interplay can be effectively captured using crystal plasticity theory.

Using various crystal plasticity models, this thesis aims to elucidate and predict the evolution of heterogeneous stress and strain fields across different length scales. In Chapter 3, this investigation is conducted at the macroscopic scale for a single-phase material. Chapter 4 extends the investigation at that scale to multilayered systems composed of two distinct alloys. Finally, Chapter 5 transitions to the microscopic scale to study the complex interactions among individual grains within a polycrystal. Understanding these inter-granular interactions is particularly pertinent, as it provides a critical assessment of the underlying hypotheses governing the ALAMEL model, which is extensively employed in Chapters 3 and 4. Accordingly, the primary objectives of this work are formulated around the following three research questions:

How does a through-thickness texture gradient, induced by extrusion, influence the development of heterogeneous stress fields during subsequent plastic processing?

During the extrusion of aluminium alloys, a through-thickness texture gradient frequently develops, partitioning the cross-section into three distinct regions, each characterized by a specific crystallographic texture. The plastic co-deformation of these distinct layers during subsequent forming generates a highly heterogeneous stress field. However, the extent to which this initial texture gradient governs the evolution of stress heterogeneity during subsequent forming operations remains insufficiently explored. A better understanding of the origin of this heterogeneous stress field is crucial to preserve the structural integrity and mechanical performance of the final components.

What is the strain heterogeneity across the thickness of roll-bonded multilaminates, and how can this strain gradient be revealed?

In single-phase metallic materials, it is well established that rolling induces a through-thickness strain gradient arising from the non-uniform deformation paths imposed by the roll-gap geometry and the friction induced with the rolling mill. In contrast, roll-bonded multilaminates are expected to generate unconventional through-thickness strain gradients due to the constrained co-deformation of materials with contrasting mechanical properties. Controlling the plastic strain accommodated by each individual layer is therefore essential for preserving good macroscopic mechanical response, particularly

with regard to ductility and fracture toughness. In this context, the ability to reveal and quantitatively assess strain heterogeneity across the thickness provides critical insight for optimizing roll-bonding parameters and enhancing the structural integrity of multilayers.

How does proximity to crystalline interfaces affect plastic deformation, and how can these effects be incorporated into a CPFEM framework?

Even when the macroscopic deformation field is uniform, the microscopic deformation field within polycrystals is highly heterogeneous. Indeed, stress equilibrium and strain compatibility must be satisfied at every crystalline interface, which leads to the emergence of heterogeneous strain fields. Consequently, the strain within a grain is expected to depend on the distance to crystalline interfaces, such as grain boundaries, triple junctions, and quadruple points. Understanding this relationship is essential not only for elucidating the origin of microscopic heterogeneity but also for incorporating these effects into a CPFEM framework, which is particularly relevant in simulations where heterogeneity plays a critical role in phenomena such as fracture.

Internal stresses in an extruded aluminium alloy sheet

3

Industrial metal forming processes are widely employed to produce sheet materials with prescribed geometries. These processes generally induce complex and spatially heterogeneous microstructural features, such as variations in grain size, grain morphology, and phase distribution. While these heterogeneities have been extensively investigated and optimized to enhance mechanical performance (Jacques et al., 1998; Qin et al., 2019; Habibi et al., 2021), forming operations also generate process-specific crystallographic textures. These textures influence the anisotropic mechanical response of the metallic sheets. Assuming a uniform texture across the sheet, the stress field generated during subsequent plastic deformation remains uniform across the sheet thickness. However, certain forming processes induce through-thickness texture gradients. The presence of such a texture gradient raises questions regarding its specific mechanical impact. Therefore, this chapter investigates the relationship between pre-existing texture gradients and the development of heterogeneous stress fields during subsequent plastic deformation, specifically in the context of a texture gradient generated during extrusion.

The chapter is organized as follows. The current state of knowledge regarding texture heterogeneity in extruded aluminium alloy sheets and its possible relationship with the development of a non-uniform stress field is reviewed in the introductory section. The material under investigation and the experimental characterization techniques are described in Section 3.2. The numerical frameworks employed for the analyses are presented in Section 3.3. In Section 3.4, the plastic anisotropy associated with the macroscopic texture, as well as that associated with the different textures measured across the thickness, is predicted and compared. The development of internal stresses is also assessed. The results are discussed in Section 3.5, followed by the conclusions of the chapter.

This chapter is the result of a collaboration with Clément Pot and Professor Philippe Bocher from École de technologie supérieure (ÉTS) in Montréal, Canada.

3.1 Introduction

Extrusion of metallic billets is a widely used metal-forming process for manufacturing sheets with prescribed cross-sectional geometries (see the schematic representation in Figure 3.1). However, post-processing operations performed on flat extruded aluminium alloy sheets revealed the development of significant internal stresses following subsequent plastic deformation. Earlier investigations have, for instance, reported localized regions of contraction and tension across the sheet thickness after additional straining, indicating the presence of residual stresses (Chen et al., 2018). A fundamental understanding of the origin, magnitude and direction of these stresses in extruded aluminium alloy sheets is therefore essential, particularly when further forming operations are required.

Flat-die extrusion of aluminium alloys often produces thick plates with complex and heterogeneous microstructures exhibiting a composite-like architectures. Near the surfaces of the flat die, peripheral coarse grains (PCGs), as illustrated in Figure 3.2, are commonly observed, characterized by crystallographic axes close to $\langle 111 \rangle$ aligned with the transverse direction TD (in-plane direction perpendicular to the extrusion direction ED) (Eivani et al., 2020; Negrozio et al., 2025a; Liu et al., 2026). These orientations, associated with S $\{123\}\langle 634 \rangle$ and Brass $\{011\}\langle 211 \rangle$ components, are generally formed by discontinuous recrystallization driven by frictional interactions at the die-material interface. In contrast, the central region of the sheet generally contains finer grains with $\langle 100 \rangle // \text{ED}$ orientations, composed mainly of Cube $\{001\}\langle 100 \rangle$ and Goss $\{011\}\langle 100 \rangle$ components. The Cube component is primarily formed prior to entering the extrusion die and subsequently increases its volume fraction while passing through the die section (Khadyko et al., 2016; Rousselier et al., 2012; Araki et al., 2020). Die design strongly influences these distributions (Mahmoodkhani et al., 2019; Esterl et al., 2025). For extruded sheet of AA6063, the average texture is usually dominated by the Cube orientation (Pot et al., 2023). The development of this component is promoted by Mg and Si solutes, which reduce the stacking fault energy, thereby enhancing stored strain energy and driving the preferential growth of Cube-oriented grains during recrystallization (Araki and Matsuda, 2020). By contrast, alloys such as AA6082 or Al-Zn-Mg-Zr may retain fibrous microstructure with a strong β -fibre texture under similar conditions (Pedersen et al., 2008; Park et al., 2021). PCGs are not systematically observed in these two alloys (Pot et al.). These last alloys, developing fibrous microstructure, are not studied in the present work.

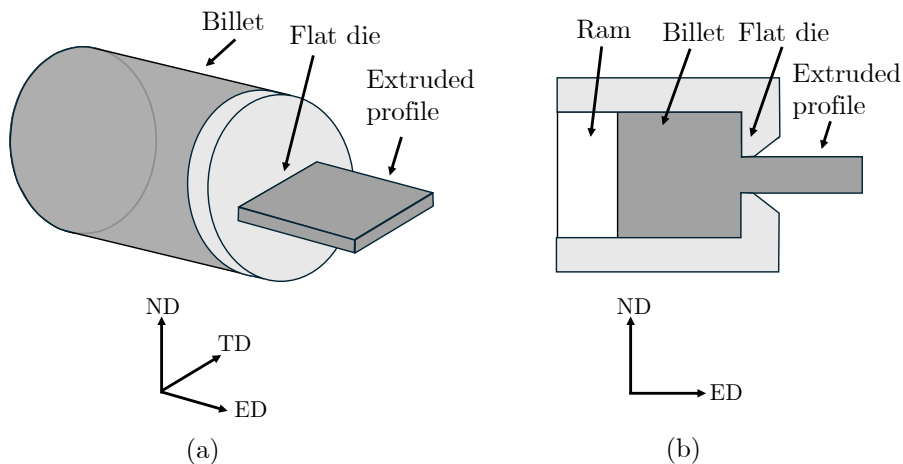


Figure 3.1: Schematic representation of the flat die extrusion process: (a) 3D view illustrating the reference coordinate system and (b) 2D cross-section along the ND-ED plane. The cross-sectional view in (b) is reproduced and adapted from Francis (2016).

The heterogeneity of texture between peripheral and central regions can give rise to stress heterogeneity between the layers if post-processing of the sheet involves plastic deformation. In aluminium alloys, crystallographic texture is the primary source of anisotropy (Oscarsson et al., 1991; Bate and An, 2004; Engler and Aegerter, 2014). Therefore, non-uniform textures are likely to host non-uniform mechanical fields. However, characterization of the distinct anisotropic behaviour of these regions has received limited attention. Experimentally, only the Lankford coefficients of the central region have been reported, leaving the plastic anisotropy of the peripheral coarse-grained (PCG) region uncharacterized (Li et al., 2005; Chen et al., 2018). A numerical study using viscoplastic self-consistent (VPSC) simulations reported that textures representative of the peripheral and central regions gave markedly different predicted R-values at 45° and 90° relative to the extrusion direction, suggesting plastic-deformation incompatibilities between layers and the potential development of internal stresses for these tensile directions (Chen et al., 2018). However, the resulting internal stress fields have received little attention beyond qualitative observations of barrelling deformation across the sheet thickness.

Several modelling strategies have been employed to predict macroscopic plastic anisotropy in extruded aluminium sheets, but none was used to analyse the development of internal stresses arising from texture gradients. A widely

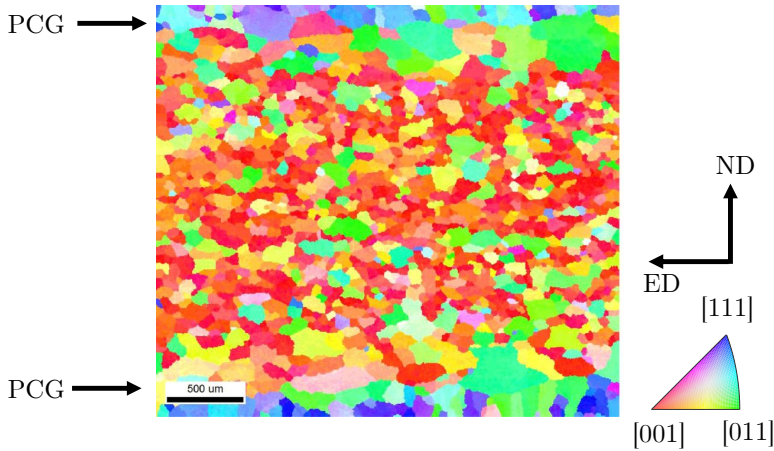


Figure 3.2: Identification of the peripheral coarse-grained (PCG) region within the ED-ND cross-section. The inverse pole figure (IPF) map is colored with respect to the transverse direction (TD). The orientation map is coming from Khadyko et al. (2016).

used approach to investigate macroscopic plastic anisotropy involves to use the measured average through-thickness texture as input for mean-field crystal plasticity models, VPSC model or crystal plasticity finite element models (CPFEM). Such approach has proven capable of reproducing experimentally observed macroscopic anisotropy without explicitly reconstructing the full texture gradient (Engler and An, 2005; Bate and An, 2004; Ghosh et al., 2015; Khadyko et al., 2016, 2017). However, these approaches assume a spatially uniform texture and thus can not capture the emergence of internal stresses induced by texture heterogeneity. Rule-of-mixtures (ROM) approaches, originally developed for clad sheets composed of dissimilar materials (Sakaki et al., 1991; Bong et al., 2024), account for the individual properties of constituent layers but are also not suited to predict the development of internal stresses. The most advanced approach, CPFEM, enables the modelling of heterogeneous textures and EBSD-based microstructural geometries. Despite its successful application to capture macroscopic behaviour, CPFEM has not yet been applied to investigate the generation of internal stresses in extruded metallic sheets exhibiting through-thickness texture heterogeneity (Bong et al., 2024; Khadyko et al., 2016).

Although the macroscopic plastic anisotropy of extruded aluminium alloys has been extensively studied, key questions remain concerning the through-thickness heterogeneity of texture. In particular, the relationship between texture gradient, internal-stress development and macroscopic anisotropy remains insufficiently unexplored. The present study addresses these gaps

through a combined experimental and numerical investigation of an extruded AA6063 sheet. Specifically, the study aims to answer the following questions:

- How significant are the internal stresses arising from the strain incompatibility between the distinct crystallographic textures characterizing the surface and central regions?
- How different are the anisotropic responses of the texture components formed during extrusion, and how do they contribute to the macroscopic anisotropy?
- Among Taylor FC, ALAMEL, and CPFEM models, which crystal plasticity model best captures both plastic anisotropy and the emergence of internal stresses?

3.2 Experimental measurements

All experimental measurements were conducted mostly by Clément Pot within the research team of Prof. Philippe Bocher from École de technologie supérieure (ÉTS) in Montréal, Canada.

This study investigated aluminium alloy AA6063 with a chemical composition given in Table 3.1. The alloy was first processed by direct-chill (DC) casting to produce a billet with an outer diameter of 101 mm. This billet subsequently underwent a homogenization heat treatment at 500°C according to a standard thermal cycle .

Prior to extrusion, the billet was preheated to 500°C. Temperature at the die exit reached approximately 535°C. The billet was extruded at a ram speed of 12 mm/s in a 90 mm wide 2.9 mm thick flat profiles, quenched by water spray immediately after exiting the extrusion die. This results in an extrusion ratio (defined as the ratio of the initial to final cross-sectional area) of 25. No post-extrusion heat treatment was applied. The profiles were stored about 2 years before the present study.

Mg	Si	Mn	Cr	Fe	Cu	Al
0.49	0.44	0.03	0.0	0.18	0.01	Bal.

Table 3.1: Nominal chemical composition of the material extruded AA6063.

To characterize the mechanical properties, micro-tensile tests were performed on specimens extracted at various orientations relative to the extrusion direction (ED). Specifically, angles of 0°, 22.5°, 45°, 67.5°, and 90° were evaluated. The specimen geometries were based on ASTM E8 standard, as illustrated

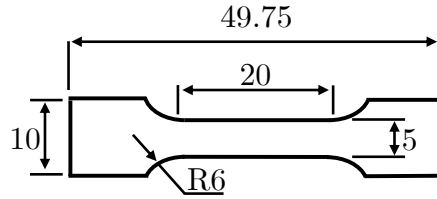


Figure 3.3: Geometry of the tensile specimen according to ASTM E8 (dimensions in mm).

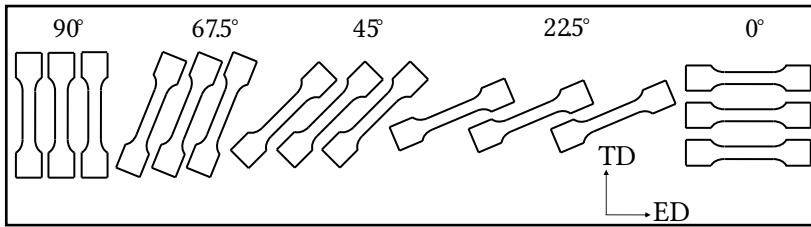


Figure 3.4: Machining plan of the tensile specimen extracted from the extruded profile. ED denotes the extrusion direction, while TD represents the transverse direction.

in Figure 3.3. The specimen machining plan is detailed in Figure 3.4. Due to the spatial and load constraints of the testing equipment - a 5 kN micro-tensile/compression module (Kammrath & Weiss GmbH, Schwerte, Germany) - the dimensions of the gauge section were modified. Accordingly, the gauge width and length were reduced to 5 mm and 20 mm, respectively. All tests were conducted at a constant macroscopic strain rate of 0.5 s^{-1} . Optical images were recorded during deformation at a frame rate of 1 per second using a Manta G504B camera (Allied Vision) and were subsequently analyzed to provide strain measurements in both the axial and transverse directions using the open-source software OpenDIC (Vanderesse et al., 2013).

Prior to micro-mechanical testing, a batch of tensile specimens was manually polished to remove a $700 \mu\text{m}$ layer from both through-thickness surfaces. This material removal was necessary to eliminate surface layers exhibiting significant crystallographic texture gradients, thereby isolating the central region of the extruded profile for characterization. The polishing procedure utilized progressive silicon carbide (SiC) grinding papers ranging from 320 to 1200 grit, followed by a final polishing stage using $3 \mu\text{m}$ and $1 \mu\text{m}$ monocrystalline diamond suspensions to achieve a mirror finish.

For microstructural characterization, an as-extruded sample was sectioned along the transverse direction-normal direction (TD-ND) plane. The observa-

tion surface was mechanically prepared using progressive silicon carbide (SiC) grinding papers (320 to 1200 grit), followed by polishing with 3 μm and 1 μm monocrystalline diamond suspensions. To ensure a surface finish suitable for electron backscatter diffraction (EBSD) analysis, the sample was subsequently electropolished at 30 V for 60 s. The electrolyte consisted of ethanol (700 mL at 95%), distilled water (120 mL), 2-Butoxyethanol (100 mL) and perchloric acid (80 mL at 60%). EBSD measurements were conducted using a Hitachi SU-70 field emission gun scanning electron microscope (FEG-SEM). Mapping was performed over an area of $2425 \mu\text{m} \times 2465 \mu\text{m}$ using a step size of 5 μm , yielding a total of 240084 data points.

Crystallographic texture analysis was performed using the MTEX toolbox (Hielscher and Schaeben, 2008). The Orientation Distribution Function (ODF) was reconstructed from discrete EBSD measurements via Kernel Density Estimation (KDE). This estimation employed a radially symmetric de la Vallée Poussin kernel with a constant half-width of 10° . To ensure statistical representativeness, the ODF calculation integrated the full dataset of indexed orientations without subsampling. The numerical computation was executed using the spectral method based on Generalized Spherical Harmonics, which optimizes the convolution efficiency for large datasets. Texture visualization was performed through ODF sections and pole figures using a stereographic projection.

Inverse pole figure (IPF) maps obtained from EBSD measurements revealed a heterogeneous distribution of crystallographic orientations across the sample thickness, as shown in Figure 3.5. Two distinct regions were identified:

1. **Central region** ($0.25th \leq z \leq 0.75th$): grains predominantly exhibited the [001] axis aligned with the extrusion direction, corresponding to the red color in the IPF map colored using the ED as the projection axis (Figure 3.5a). Note that the grains in this region did not all share the same crystallographic orientation as some grains had their [001] axes and others their [011] axes aligned with the transverse direction (TD), corresponding to the red and green colors, respectively, in the IPF map colored using the TD as the projection axis (Figure 3.5b). This region comprised approximately 1116 grains.
2. **External regions** ($z < 0.25th$ and $0.75th < z$): most grains exhibited either their [011] or [111] crystallographic axes aligned with the extrusion direction, corresponding to the green and blue colors, respectively, in Figure 3.5a. Both regions comprised approximately 469 and 389 grains.

The crystallographic textures differed a lot between the central and external regions. As depicted in Figure 3.6, the central region exhibited a strong texture, dominated by Cube {001} $\langle 100 \rangle$ and Goss {011} $\langle 100 \rangle$ components. Conversely, the orientation distribution functions (ODFs) of the two near-surface

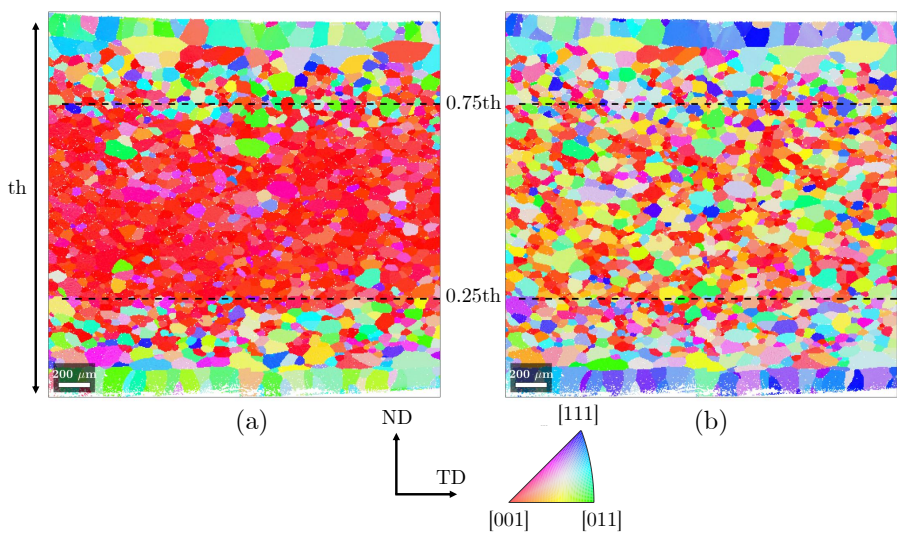


Figure 3.5: Inverse pole figure (IPF) maps of the Transverse Direction (TD) - Normal Direction (ND) cross-section. Maps are colored using (a) the extrusion direction (ED) and (b) the transverse direction (TD) as the IPF axis.

	Cube (%)	Copper (%)	Goss (%)	Brass (%)	S (%)
$z < 0.25th$	11	3	2	2	6
$0.25th < z < 0.75th$	34	1	16	3.5	5
$0.75th < z$	9	3.5	3	1	4

Table 3.2: Volume fractions of the main crystallographic texture components in the different regions. A cutoff angle of 15° around the ideal component orientations was applied to determine the fractions. z is the position along the normal direction (ND).

regions were comparable (Figure 3.7). These peripheral regions presented a notably weaker overall texture, though the Cube component remained dominant. The volume fractions of the main texture components for each regions are summarized in Table 3.2.

The combined contributions of all layers resulted in a macroscopic texture exhibiting orthorhombic symmetry, characteristic of flat-die extrusion. This texture was dominated by the Cube $\{001\}\langle 100 \rangle$ component, with minor Goss $\{011\}\langle 100 \rangle$ and S $\{123\}\langle 634 \rangle$ components. The volume fractions of texture components giving this macroscopic texture was consistent with previously reported measures for such extruded AA6063 alloys (Araki and Matsuda, 2020; Sabat et al., 2021).

Grain size also varied across the thickness. The central region contained a

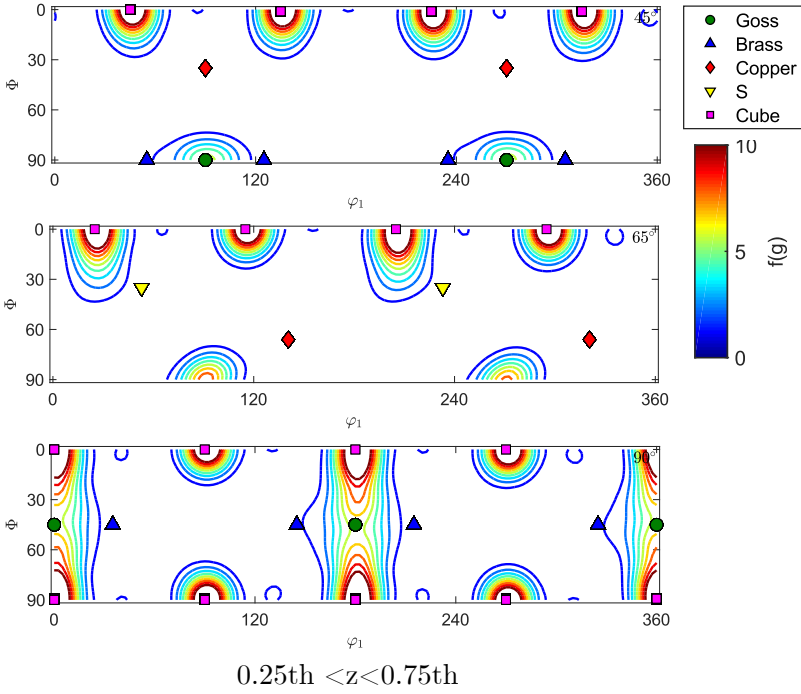


Figure 3.6: Orientation distribution functions (ODFs) of the central region. Ideal crystallographic orientations are also included for reference.

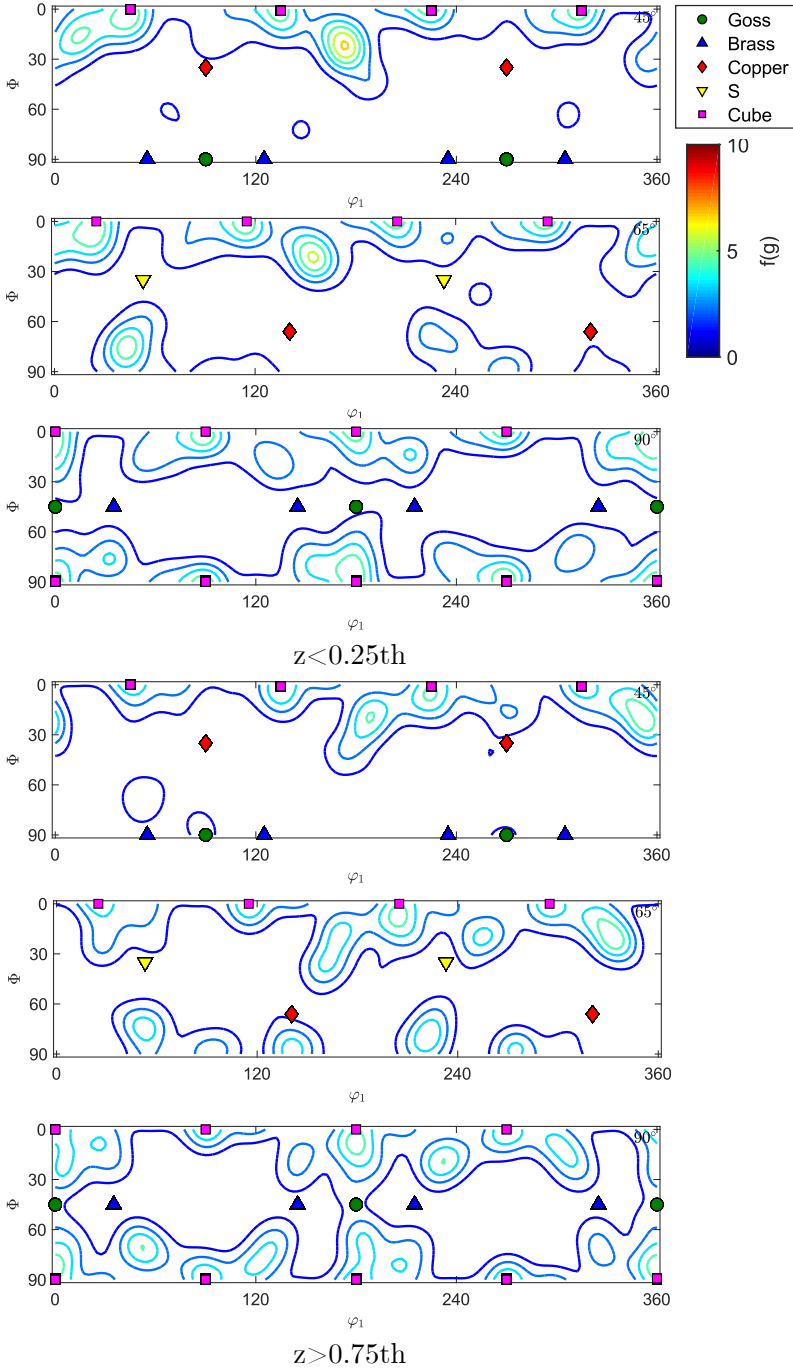


Figure 3.7: Orientation distribution functions (ODFs) of the two external regions. Ideal crystallographic orientations are also included for reference.

finer microstructure, with an average grain radius of about $40\mu\text{m}$, whereas the external layers exhibited coarser grains, with average radii of $65.3\mu\text{m}$ in the upper region and $53.3\mu\text{m}$ in the lower region.

A Vickers hardness distribution was measured on cross-sections oriented such that the extrusion direction (ED) was normal to the examined plane. Measurements were conducted using a CLEMEX microhardness tester with a step size of $400\mu\text{m}$ along both the normal (ND) and transverse (TD) directions. A load of 100 gf and a holding time of 10 s was used. The hardness values ranged narrowly between 63 and 68 HV across the thickness, yielding an average of 65 HV for both the central and surface regions. No significant hardness gradient was observed.

The cross-sections of uniaxial tensile test specimens loaded at 0° , 45° , and 90° with respect to the extrusion direction were characterized after plastic deformation. The contour of the cross-section along the specimen thickness were obtained using a Keyence VR-5200 wide-area 3D measurement system using profilometer option. The samples sides were scanned allowing to acquire the shape and waviness profiles. No filter was applied.

Residual stress measurements were performed on a Pulstec $\mu 360$ X-ray diffraction instrument equipped with a chromium source, operating at a voltage of 30 kV and a current of 1 mA, with a collimator diameter of 1 mm. Stress calculations were based on the $\{311\}$ aluminium peak. Internal stresses were measured along the loading direction and the transverse direction on the top surface (corresponding to the ED–TD plane) of uniaxial tensile specimens loaded at 0° , 45° , and 90° with respect to the extrusion direction. The Pulstec equipment uses the $\cos(\alpha)$ method to calculate the residual stresses based on the analysis of Debye-Scherrer rings (Delbergue et al., 2016). In this technique, the diffraction of X-rays by the crystal lattice generates a characteristic ring pattern on a 2D detector. While an unstressed specimen produces a perfectly circular Debye ring, the presence of residual stress induces a distortion in the ring geometry. Specifically, the lattice strain varies as a function of the azimuthal angle α along the Debye ring. Consequently, the residual stress values are derived from the slope of the linear regression of the strain versus $\cos \alpha$, measured along a quarter section of the diffraction ring. The calculation achieved by the Pulstec machine are based on only one ring measurement.

3.3 Description of the models

Three crystal plasticity models were used: two mean-field approaches (Taylor full-constraints (FC) and ALAMEL) and a full-field crystal plasticity finite element model (CPFEM). Beyond the specific modelling assumptions of each CP model, several simplifying assumptions were adopted to well identify the influence of the crystallographic texture. First, a uniform grain size was assumed through the sheet thickness, the experimentally observed gradient in grain size was therefore neglected and hardness was assumed uniform. Second, potential initial residual stresses resulting from the extrusion process were not considered.

The different CP models require, as input, a discrete set of crystallographic orientations. Consequently, discrete sets of crystallographic orientations, statistically representative of the experimental textures, were generated following the discretization method proposed by Melchior and Delannay (2006). The ODF was first integrated over a regular grid in Euler space with a step size of 5° (ϕ_1, Φ, ϕ_2) to define local orientation probabilities. These probabilities were subsequently arranged into a cumulative distribution function (CDF). The discrete orientation sampling was performed via an inverse transform sampling method. This technique ensures a discretization where the density of selected orientations is proportional to the experimental ODF. During this procedure, an orthotropic specimen symmetry was enforced. While it is recognized that the extrusion process induces shear deformations near the surfaces - thereby deviating from strict orthotropy - this idealized symmetry was retained as a first-order approximation. This choice is supported by the relatively weak experimental texture of the external layers, which is predominantly characterized by the highly symmetric Cube component (Figure 3.7). For simulations predicting macroscopic plastic anisotropy, the discretization was performed from the ODF of the macroscopic texture measured experimentally. Figure 3.8 compares the experimental pole figures with that obtained from the discretized average through-thickness texture used in the mean-field simulations, showing the close correspondence between them. The resulting volume fractions of the main texture components are reported in Table 3.3, further confirming the good agreement with the experimental distribution. The same sampling procedure was applied to generate statistically representative orientation sets for the external and central regions.

For both mean-field models (Taylor FC and ALAMEL), simulations were conducted using an aggregate of 10000 grains. This sample size was selected to ensure a statistically representative sampling of the orientation space (Van Houtte et al., 2005). When macroscopic plastic anisotropy was

	Cube (%)	Copper (%)	Goss (%)	Brass (%)	S (%)
Experimental texture	22	2	9	2.5	5
Sampled texture (Mean-Field models)	22	2	8.5	2.5	5
Sampled texture (CPFEM)	21	2	8.5	2.5	5

Table 3.3: Volume fractions of the main crystallographic texture components. A cutoff angle of 15° around the ideal component orientations was applied to determine the fractions.

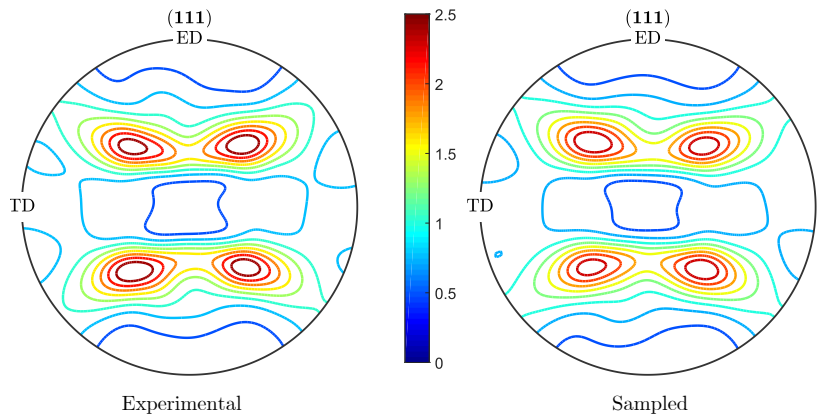


Figure 3.8: $\{111\}$ Pole figures of the experimental macroscopic texture measured by EBSD (~ 2000 grains) and of the textures generated for the mean-field models (10000 grains). ED is the extrusion direction and TD is the transverse direction.

Crystal lattice	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	τ_{c0} [MPa]	Γ_0 [-]	n [-]	m [-]	$\dot{\gamma}_0$ [1/s]
FCC	107.3	60.9	28.3	35	0.021	0.3	100	0.01

Table 3.4: Material parameters calibrated to reproduce the tensile response along the extrusion direction measured experimentally. The same parameters were used in both mean-field and CPFEM simulations.

investigated, all grains were assigned crystallographic orientations sampled from the macroscopic experimental texture. In contrast, for the analysis of internal stress development, half of the grains were assigned orientations sampled from the external texture and the remaining half from the central texture, thereby incorporating the through-thickness texture heterogeneity.

In CPFEM simulations, the geometry reproduced a representative volume of the tensile specimen, with dimensions of 5 mm in width, 2.5 mm in thickness, and 5 mm in length. Half of the total thickness was attributed to the external region, corresponding to a ratio $th_{ext}/th_{tot} = 0.5$. The mesh contained of 32000 C3D8 brick elements, each representing a grain and therefore hosting a single crystallographic orientation. The external layers contained 8000 elements each, while the central region comprised 16000 elements. For CPFEM simulations dedicated to investigate the macroscopic plastic anisotropy, each element was assigned a crystallographic orientation sampled from the average texture, irrespective of its position through the thickness. Indeed it was shown that, for studying macroscopic plastic anisotropy, reproducing texture distribution through thickness and grain shape of the microstructure did not significantly improve predictions of macroscopic plastic anisotropy, while increasing the complexity of the material assignment as observed by Khadyko et al. (2016). To investigate the development of internal stresses, the through-thickness variation of texture was explicitly taken into account. In this case, each element was assigned a single orientation sampled either from the external or the central texture, according to its spatial location, as illustrated in Figure 3.10.

Each grain was modelled as a face-centered cubic (FCC) crystal, deforming plastically by dislocation glide on the $\{111\} \langle 110 \rangle$ slip systems. While the elastic constants were adopted from Hosford (1993), the hardening parameters were identified through an iterative calibration procedure using CPFEM, designed to reproduce the experimental macroscopic response under uniaxial tension along the extrusion direction, as illustrated in Figure 3.9. These parameters, reported in Table 3.4, were used for both mean-field and CPFEM simulations.

Experimentally, plastic anisotropy was characterized by performing tensile

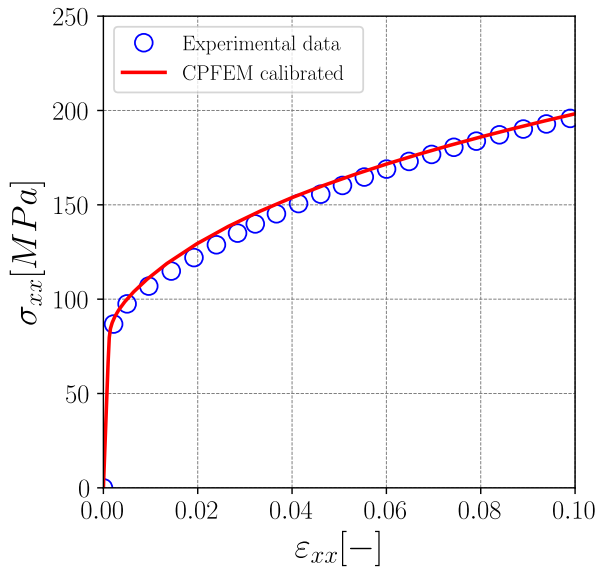


Figure 3.9: Comparison between the experimental uniaxial tensile response and the numerical prediction. The simulation employs the calibrated material parameters provided in Table 3.4, with the loading axis aligned parallel to the extrusion direction (ED).

tests at various angles within the extrusion plane, ranging from the extrusion direction toward the transverse direction (the plane normal being the normal direction, ND). In the simulations, an equivalent procedure was implemented by rotating the polycrystal instead of changing the loading direction. Specifically, all grains were rotated around the normal direction by incrementally increasing the first Euler angle φ_1 in steps of 5° , while the tensile loading direction was kept fixed along the X -direction. This approach ensures direct correspondence with the experimental testing orientations while maintaining consistent boundary conditions in the simulations. Rotations of 22.5° and 67.5° were also applied to allow direct comparison with experiments.

The macroscopic deformation imposed on the computational domain Ω corresponded to uniaxial tension along the X -direction. To reflect the physical boundary conditions of a standard experimental tensile test, macroscopic shear deformations were constrained to zero. This kinematic constraint accounts for the rigid clamping of the specimen within the testing machine, which restricts both macroscopic shear and rigid body rotations. Consequently, only the axial deformation component was prescribed. The perpendicular directions were left unconstrained to allow for natural contraction, and their corresponding macroscopic stress components were prescribed as zero. These boundary conditions can be expressed as:

$$\langle \mathbf{F} \rangle_\Omega = \begin{pmatrix} 1.1 & 0 & 0 \\ 0 & ? & 0 \\ 0 & 0 & ? \end{pmatrix} \quad \langle \boldsymbol{\sigma} \rangle_\Omega = \begin{pmatrix} ? & ? & ? \\ ? & 0 & ? \\ ? & ? & 0 \end{pmatrix}$$

Here, “?” denotes components that were not prescribed and therefore determined by the model. In CPFEM simulations, surfaces normal to the X -direction (defined as the tensile direction) were always constrained to remain planar during deformation while surfaces normal to the Y -direction and Z -direction were either kept planar or left free, depending on whether barreling effects were to be explored.

To evaluate the development of residual stresses, an elastic unloading phase was introduced into the CPFEM simulations via a relaxation step. In this step, the macroscopic stress tensor was prescribed as zero, and all deformation components were left completely unconstrained to allow for full elastic recovery:

$$\langle \mathbf{F} \rangle_\Omega = \begin{pmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & ? \end{pmatrix} \quad \langle \boldsymbol{\sigma} \rangle_\Omega = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

This relaxation procedure cannot be performed within the mean-field models as the same velocity gradient is used for both layers. Indeed, during the

relaxation step, the deformations of the external and central regions in the X -direction and Y -directions are expected to be identical, whereas the deformation in the Z -direction may differ, as the layers do not mechanically interact along this direction. However, in mean-field simulations, the same velocity gradient is applied uniformly to all grains (for Taylor FC) or 2-grains (for ALAMEL), irrespective of their position, which would lead to an inaccurate prediction of the internal stresses. Consequently, internal stresses were estimated by subtracting the macroscopic stress $\langle \sigma \rangle_\Omega$ from the average stress of all grains associated with the same texture layer $\langle \sigma \rangle_{layer}$.

A direct comparison between the internal stresses predicted by CPFEM and those obtained from mean-field models is only meaningful when the CPFEM simulations enforce planar boundary conditions on the surfaces normal to the loading direction. These conditions prevent stress relaxation associated with barreling, a phenomenon that mean-field models are not able to reproduce.

In CPFEM, a third step was designed to mimic material removal along the thickness in removing successive layers of elements. In practice, it means that Abaqus stored the forces exerted by the elements to be removed on the residual part and then gradually ramped down these forces to zero to ensure smooth relaxation of the model. Such simulation can not be performed with mean-field models.

To characterize the anisotropic response of the sheet, four metrics were evaluated: the Lankford coefficient (R -value), the strain ratio (q), the flow stress ratio, and the Taylor factor. These parameters were determined via uniaxial tensile tests performed at various orientations, defined by the angle ψ between the extrusion direction (ED) and the tensile axis. The testing orientations ranged from the ED ($\psi = 0^\circ$) to the transverse direction (TD, $\psi = 90^\circ$). In the adopted coordinate system, the x -axis is aligned with the tensile direction. Consequently, the Lankford coefficient is defined as the ratio of the in-plane transverse plastic strain rate to the through-thickness plastic strain rate as $d\dot{\epsilon}_{yy,p}/d\dot{\epsilon}_{zz,p}$. Similarly, the strain ratio, q , is defined as $-d\dot{\epsilon}_{xx,p}/d\dot{\epsilon}_{zz,p}$. Note that under the assumption of plastic incompressibility ($\text{tr}(\dot{\epsilon}^p) = 0$), these two parameters are intrinsically coupled. The directional dependence of the material strength is captured by the flow stress ratio. This is expressed as the yield stress measured at an orientation ψ , normalized by the reference yield stress obtained in the transverse direction as $\sigma_{yield}(\psi) / \sigma_{yield}(90^\circ)$. In addition, the volume-averaged Taylor factor, denoted by M , was evaluated for each loading direction. This parameter provides a micromechanical measure of the resistance to plastic deformation and is computed by averaging, over the polycrystalline aggregate, the ratio of the accumulated crystallographic shear

rate to the equivalent plastic strain rate for each grain, as $M = \left\langle \frac{\sum_{\alpha} |\dot{\gamma}^{\alpha}|}{\dot{\epsilon}_{eq}^p} \right\rangle_{\Omega}$. All quantities were evaluated at a longitudinal strain of $\epsilon_{xx} = 0.095$. Finally, to provide a global assessment of the sheet's anisotropy, the normal anisotropy coefficient ($\bar{R}$) and the planar anisotropy coefficient (ΔR) were calculated as: $\bar{R} = \frac{R0+2R45+R90}{4}$ and $\Delta R = \frac{R0-2R45+R90}{2}$.

3.4 Results

3.4.1 Macroscopic plastic anisotropy

In Figure 3.11, the predicted Lankford curves, using the average through-thickness texture, showed a convex profile. All models predicted similar Lankford curves, with a minimum R -value around 35° – 40° and values ranging from 0.14 to 1.66. Experimentally, the R -values also exhibited a convex trend, but the minimum could not be precisely located due to the limited number of orientations tested. The experimental values stayed below 1, ranging between 0.34 and 0.81, corresponding to a low planar anisotropy coefficient of 0.1. Numerical predictions of the planar anisotropy coefficient were slightly higher, ranging between 0.67 and 0.82, due to underestimation of $R45$ and overestimation of $R90$ by the different models. However, the models predicted the normal anisotropy coefficient reasonably similar to the one measured experimentally. The average error with the experimental R -values, presented in Table 3.5, indicates that no single model outperformed the others in predicting the Lankford coefficients.

	R0	R22.5	R45	R67.5	R90	error	$\bar{R}$	ΔR
Exp.	0.37	0.34	0.49	0.69	0.81	0	0.54	0.1
Taylor FC	0.37	0.26	0.19	0.62	1.66	0.26	0.6	0.82
ALAMEL	0.44	0.3	0.3	0.66	1.51	0.21	0.64	0.67
CPFEM	0.42	0.29	0.27	0.66	1.56	0.22	0.63	0.72

Table 3.5: Experimental and simulated Lankford coefficients $R\psi$ at different orientations ψ . error is the average error with the experimental results $(\sum_{\psi} |R\psi - R\psi_{\text{exp}}|)/n$, $\bar{R}$ the normal anisotropy coefficient, and ΔR the planar anisotropy coefficient.

As presented in Figure 3.11, the anisotropy of the material also influenced the tensile stress required to achieve a given strain. The planar anisotropy of tensile stress was examined using the flow stress ratio. As for the Lankford coefficient, predictions from all numerical models were very similar. The flow stress ratio decreased slightly up to 22.5° , then increased to a maximum around

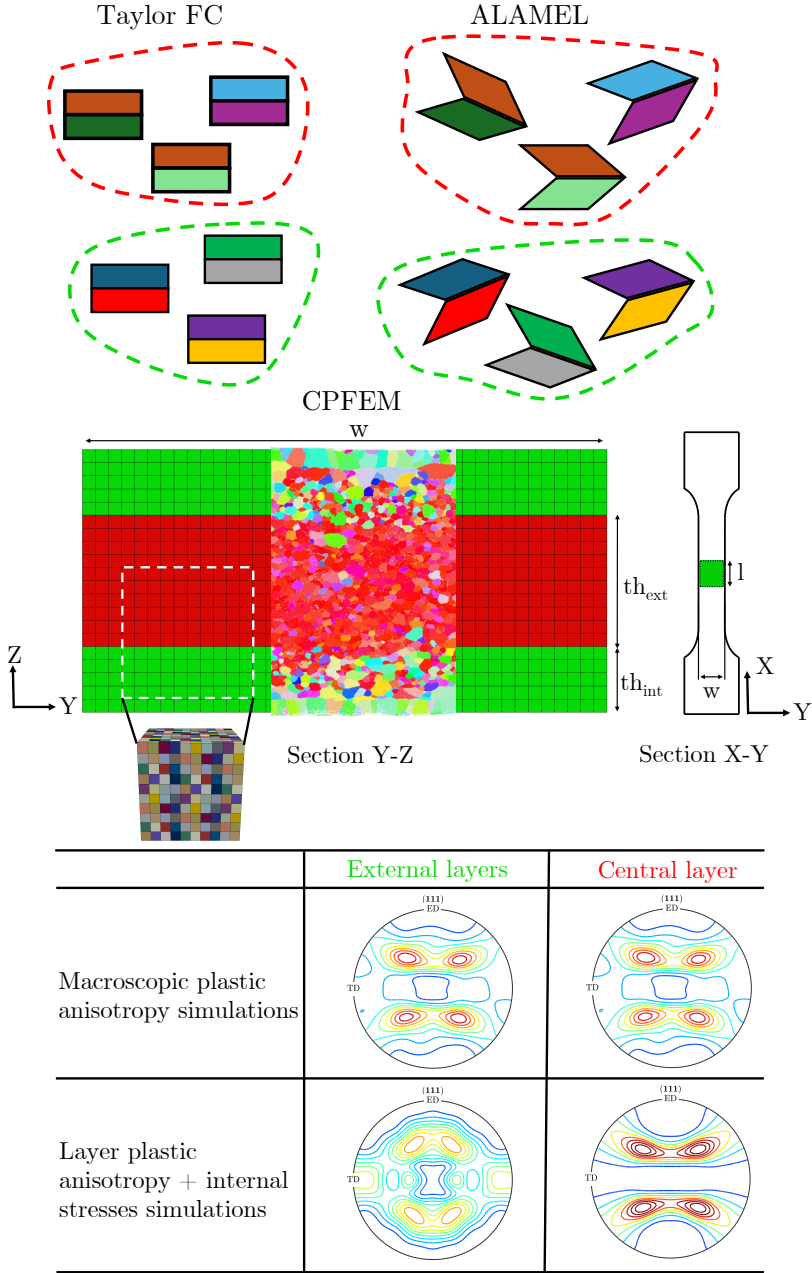
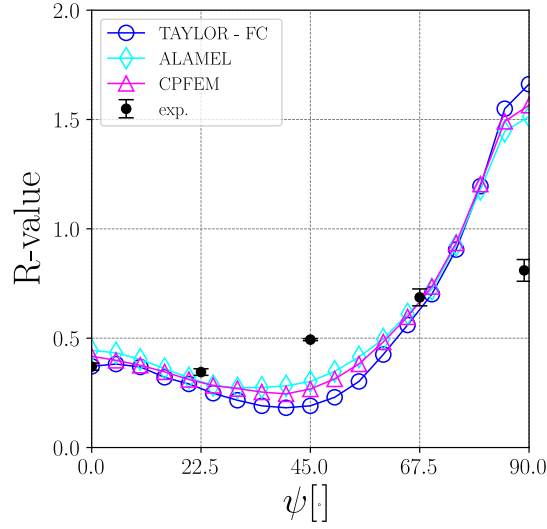
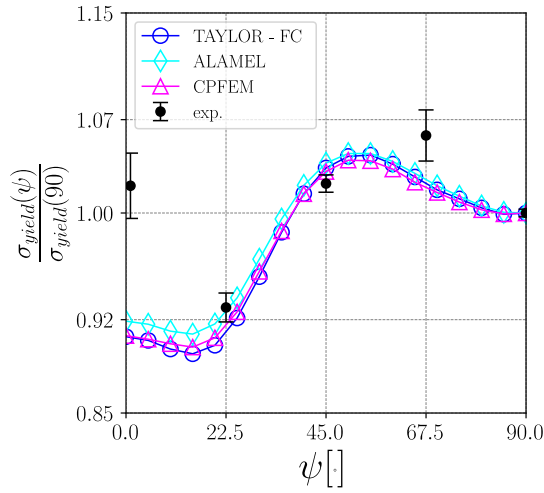


Figure 3.10: Illustration of the crystal plasticity models employed. In each model, individual grains are assigned either to the central layer (highlighted in red) or to the external layer (highlighted in green). The crystallographic orientations attributed to each layer depend on the specific simulation objective. For the CPFEM model, the representative volume has dimensions $th_{int} = 0.625$, $th_{ext} = 1.25$, $W = 5$ and $l = 5$.



(a)



(b)

Figure 3.11: Macroscopic anisotropic response: (a) evolution of the Lankford coefficients ($R\psi$) and (b) flow stress ratios, both evaluated at a longitudinal true strain of $\varepsilon_{xx} = 0.095$. Results are presented as a function of the orientation angle ψ relative to the extrusion direction (ED).

$\frac{\sigma_{yield}(\psi)}{\sigma_{yield}(90^\circ)}$	0°	22.5°	45°	67.5°	90°
Exp.	1.02	0.93	1.02	1.06	1
Taylor FC	0.91	0.91	1.03	1.02	1
ALAMEL	0.92	0.93	1.04	1.03	1
CPFEM	0.91	0.91	1.03	1.02	1

Table 3.6: Flow stress ratio measured experimentally and predicted by the different CP models. $\sigma_{yield}(\psi)$ corresponds to the tensile stress required to reach $\varepsilon_{xx} = 0.095$ when the tensile axis is oriented at an angle ψ to the extrusion direction.

45°–50°, and finally decreased again. These variations ranged between 0.91 and 1.04. Experimental measurements of the flow stress ratio exhibited a very similar evolution with a range range between 0.93 and 1.06. The comparison between experimental measurements and numerical predictions of the flow stress ratio is summarized in Table 3.6. This good agreement is further confirmed by the analysis of the yield locus in the extrusion–transverse (ED–TD) plane. As shown in Figure 3.12, the von Mises and Hill yield criteria were calibrated using the experimental data. The von Mises yield locus was calibrated solely based on the yield stress in the extrusion direction $\sigma(0^\circ)$, whereas the Hill yield locus was identified using three Lankford coefficients ($R0$, $R45$, $R90$) together with the tensile yield stress $\sigma(0^\circ)$, following the methodology proposed in Safaei and Waele (2013). Numerical predictions obtained with the different crystal plasticity models were also included and are found to closely follow the Hill yield locus, demonstrating that the models adequately capture the anisotropic yielding response. The minor discrepancies observed between the experimental yield locus and the numerical predictions are attributed to the limited number of parameters available for calibrating the Hill yield locus but also because of the use of Lankford coefficients for the calibration, which may introduce additional inaccuracies compared with calibrations based directly on yield stress measurements (Khalfallah et al., 2015; Mu et al., 2022).

3.4.2 Deformations incompatibilities across the thickness

In this section, for the sake of clarity, only the predications obtained with ALAMEL model are presented, as the CPFEM and Taylor FC models produced results very similar to those obtained with ALAMEL.

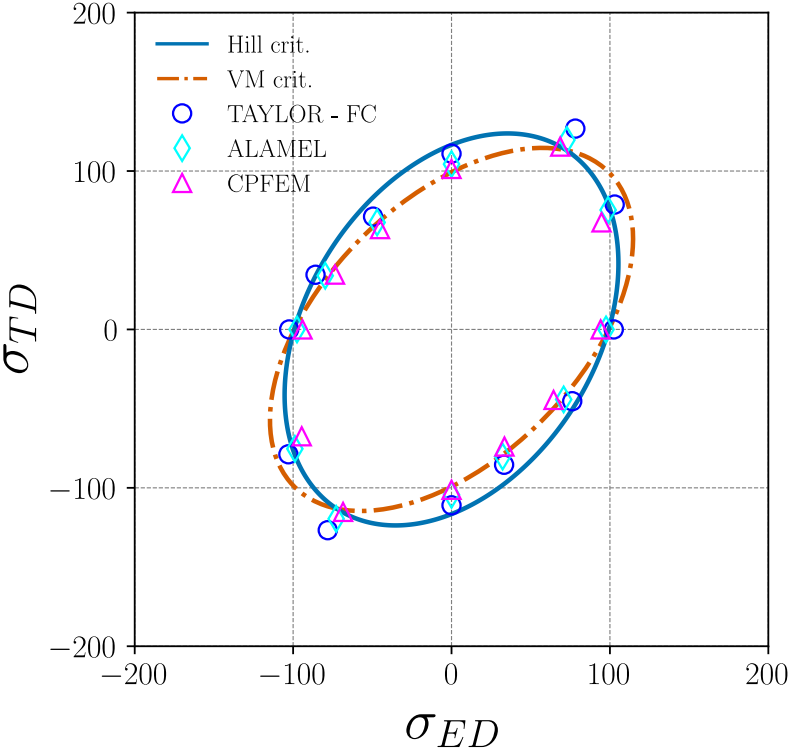


Figure 3.12: Yield loci in the ED-TD plane. Experimental data were used to calibrate the Von Mises and Hill criteria.

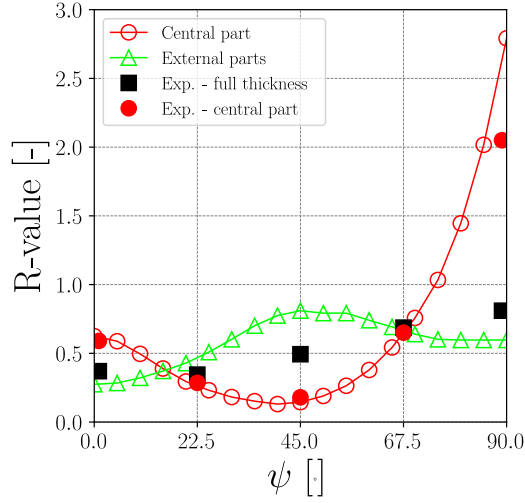
	R0	R22.5	R45	R67.5	R90	error	$\bar{R}$	ΔR
Exp. - full thickness	0.37	0.34	0.49	0.69	0.81	-	0.54	0.1
Exp. - $0.25th < z < 0.75th$	0.59	0.28	0.18	0.65	2.05	-	0.75	1.14
ALAMEL - $0.25th < z < 0.75th$	0.62	0.27	0.15	0.64	2.79	0.16	0.93	1.55
ALAMEL - $z < 0.25th$ and $0.25th < z$	0.27	0.46	0.81	0.66	0.6	-	0.62	-0.19

Table 3.7: Experimental and simulated Lankford coefficients $R\psi$ at different orientations ψ for each region of the section. error is the average error with the experimental results ($\sum_{\psi} |R\psi - R\psi_{exp}|$)/n, $\bar{R}$ the normal anisotropy coefficient, and ΔR the planar anisotropy coefficient.

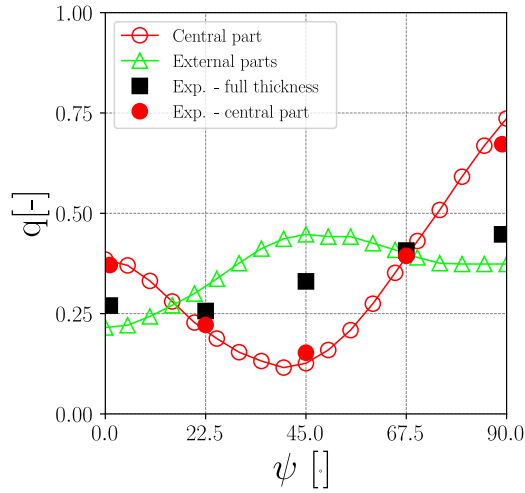
3.4.2.1 Plastic anisotropy related to the different textures

The plastic anisotropy associated with the textures of the bulk and the surface layers, respectively, was found to be very different. The distribution of the strain ratios (Lankford coefficients and the q -values) are presented in Figure 3.13. For the central part, the Lankford curve had a convex shape, with a minimum value of 0.15 at approximately 45° and a maximum of 2.8 at 90° . Experimental data for the central part obtained from the thinned samples were also added in Figure 3.13 and showed very good agreement with the predictions. The direct comparison between the measured and predicted values is given in Table 3.7. For the central part, the average error with the experimental results was even smaller than the corresponding error using the through-thickness average texture. In contrast, the external layers displayed a concave trend, with a narrower variation range: the Lankford coefficient varied between 0.27 and 0.81, reaching its maximum at 45° relative to the extrusion direction. Note that the experimentally measured coefficients for the full thickness always fell between the predictions of the central and external layers. It is interesting to note that the Lankford curves of the two layers intersected at approximately 15° and 67.5° , which thus correspond to loading direction for which the plastic anisotropy is uniform across the sheet thickness. The values at the intersections were close to experimental macroscopic R -values measured at 22.5° and 67.5° . The corresponding q -values are shown in Figure 3.13b, following the same trends as the Lankford curves.

The planar anisotropy of flow stress ratio for the central and external layers is presented in Figure 3.14a. In the central layer, the predicted ratio remained constant, around 0.92, up to approximately 22.5° , then increased to about 1.12 near 55° , before decreasing again to 1. It is interesting to note that the experimentally measured flow stress ratio for the central layer exhibited a similar evolution and comparable magnitude to the predictions, except at 0° , where the model significantly underestimated the flow stress ratio. Specifically, ALAMEL predicted a flow stress ratio of 0.92, whereas the experimental measurement yielded a value of 1.11. The predicted Taylor factor evolution

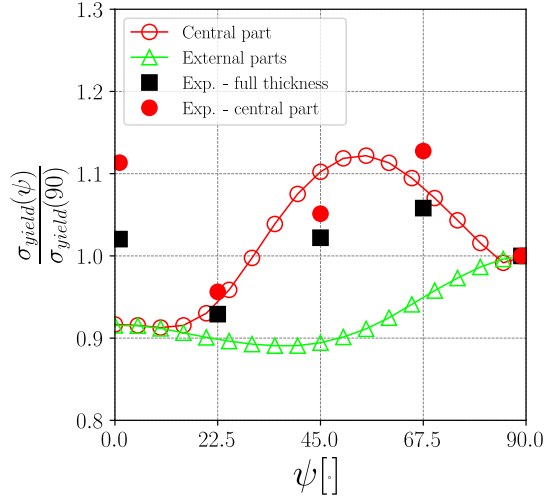


(a)

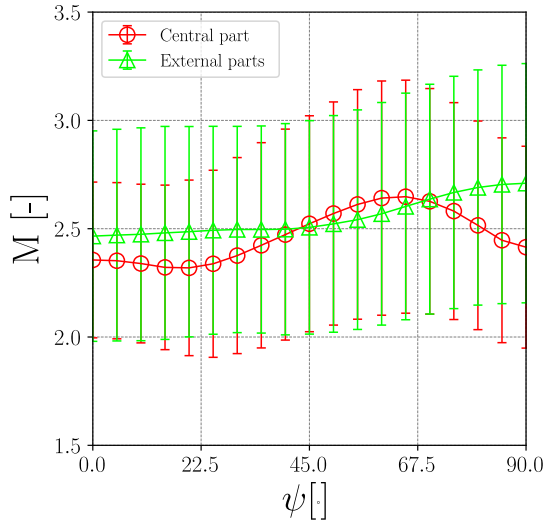


(b)

Figure 3.13: Layer-specific anisotropic responses: (a) evolution of the Lankford coefficients ($R\psi$) and (b) q -value, both evaluated at a longitudinal true strain of $\varepsilon_{xx} = 0.095$. Results are presented as a function of the orientation angle ψ relative to the extrusion direction (ED).



(a)



(b)

Figure 3.14: Layer-specific planar anisotropy: (a) flow stress ratio $\sigma(\psi)/\sigma(90^\circ)$ and (b) Taylor factor M , both evaluated at a longitudinal true strain of $\varepsilon_{xx} = 0.095$. Results are presented as a function of the loading angle ψ relative to the extrusion direction (ED).

closely followed the predicted flow stress ratio in the central part, as shown comparing Figures 3.14a and 3.14b. For the external layers, the flow stress ratio varied only slightly around 0.89 between 0° and 45° , and then increased moderately up to reaching 1. The corresponding Taylor factor showed also a similar distribution, with limited variation up to 45° , followed by a gradual increase to its maximum at 90° .

Exactly like the Lankford coefficient, the experimentally measured flow stress ratio fell between the predictions for the two layers. Only at 0° , the experimental measurement exceeded the predictions. At this orientation, the two layers had the same predicted ratio of 0.92 suggesting that the overall macroscopic ratio was similar. However, the experimentally determined value for the full thickness was 1.02, indicating a noticeable deviation from the model predictions for this loading direction.

3.4.2.2 Changing the weights of the two layers

Volume fraction

One possible reason for the slight mismatch between simulations and experiments is the relative volume fraction of the external and central regions. Preliminary observations suggested that each region contributes approximately 50% of the total thickness. However, since the boundary between the layers is not sharply defined, these proportions may not be exactly equal. To assess how variations in this fraction influence the macroscopic plastic anisotropy, several simulations were performed with different proportions of the two layers:

- $V_{ext}/V_{tot} = 0.5$
- $V_{ext}/V_{tot} = 0.6$
- $V_{ext}/V_{tot} = 0.7$

In Figure 3.15, the resulting macroscopic anisotropy showed that increasing the relative fraction of the external texture further improved the prediction of the Lankford coefficient, particularly at 90° , where R_{90} progressively approached the experimental value. The average error in the Lankford coefficients at each orientation decreased with a higher volume fraction of the external parts, whereas the flow stress ratio remained essentially unchanged. The experimentally observed flow stress ratio greater than unity at 0° remained the main difference with the experimental results. Overall, the best agreement with the experimental data was obtained when the external layer occupied more than 50% of the total volume.

	R0	R22.5	R45	R67.5	R90	error	$\frac{\sigma(0^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(22.5^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(45^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(67.5^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(90^\circ)}{\sigma(90^\circ)}$
Exp. - full thickness	0.37	0.34	0.49	0.69	0.81	-	1.02	0.93	1.02	1.06	1
ALAMEL - $V_{ext}/V_{tot} = 0.5$	0.37	0.33	0.39	0.65	1.3	0.13	0.91	0.91	1	1	1
ALAMEL - $V_{ext}/V_{tot} = 0.6$	0.35	0.36	0.47	0.65	1.13	0.08	0.91	0.91	0.98	0.99	1
ALAMEL - $V_{ext}/V_{tot} = 0.7$	0.33	0.37	0.55	0.64	0.95	0.06	0.91	0.9	0.95	0.98	1

Table 3.8: Effect of the volume fraction of the external parts V_{ext}/V_{tot} on the macroscopic predictions of the Lankford coefficient ($R\psi$) and flow stress ratio $\left(\frac{\sigma_{yield}(\psi)}{\sigma_{yield}(90^\circ)}\right)$. error is the average error with the experimental results $(\sum_\psi |R\psi - R\psi_{exp}|)/n$.

Relative strength

As the grain size was heterogeneous, the relative strength of the constituent layers is another key parameter likely to influence the macroscopic anisotropy. A harder layer is likely to have a stronger influence on the overall response. To investigate this effect, different critical resolved shear stresses (CRSS) were assigned to the external and central layers, since the yield stress is directly controlled in crystal plasticity models by the CRSS. The following configurations were studied:

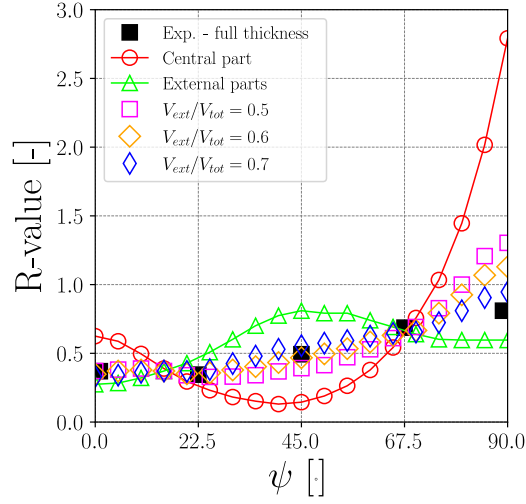
- $\tau_{c,ext}/\tau_{c,cent} = 1$
- $\tau_{c,ext}/\tau_{c,cent} = 1.5$
- $\tau_{c,ext}/\tau_{c,cent} = 2$

In all simulations that considered both textures, 50% of the crystals were assigned the central texture, while the remaining 50% were assigned the external texture.

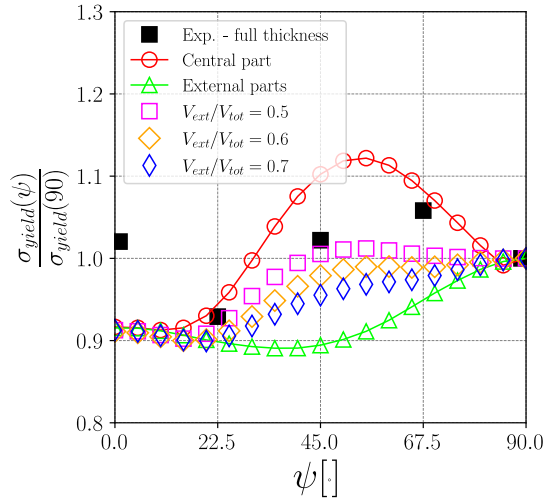
Figure 3.16 shows that increasing the CRSS of the external layers systematically improved the prediction of the Lankford coefficients without inducing large discrepancy between the predicted and experimentally measured flow-stress ratios. The best agreement with experimental results was obtained when the CRSS of the external layer was 1.5 times higher than that of the central layer, as summarized in Table 3.9.

	R0	R22.5	R45	R67.5	R90	error	$\frac{\sigma(0^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(22.5^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(45^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(67.5^\circ)}{\sigma(90^\circ)}$	$\frac{\sigma(90^\circ)}{\sigma(90^\circ)}$
Exp. - full thickness	0.37	0.34	0.49	0.69	0.81	-	1.02	0.93	1.02	1.06	1
ALAMEL - $\tau_{c,ext}/\tau_{c,cent} = 1$	0.37	0.33	0.39	0.65	1.3	0.13	0.91	0.91	1	1	1
ALAMEL - $\tau_{c,ext}/\tau_{c,cent} = 1.5$	0.34	0.35	0.47	0.66	1.12	0.08	0.91	0.91	0.98	0.99	1
ALAMEL - $\tau_{c,ext}/\tau_{c,cent} = 2$	0.32	0.36	0.53	0.64	1.03	0.08	0.91	0.9	0.96	0.98	1

Table 3.9: Effect of differences in critical resolved shear stress (τ_c) between internal and external regions on the macroscopic predictions of the Lankford coefficient $R\psi$ and flow stress ratio $\left(\frac{\sigma_{yield}(\psi)}{\sigma_{yield}(90^\circ)}\right)$. error is the average error with the experimental results $(\sum_\psi |R\psi - R\psi_{exp}|)/n$.

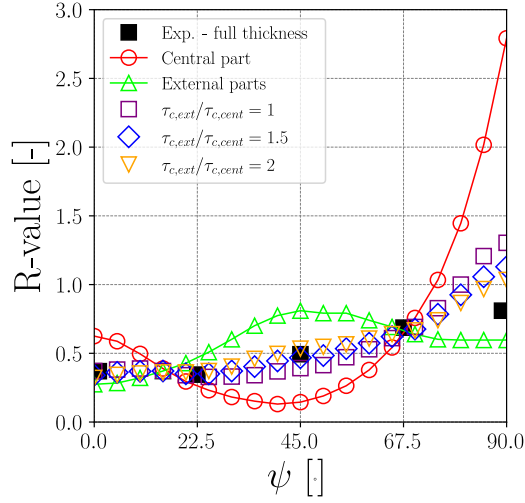


(a)

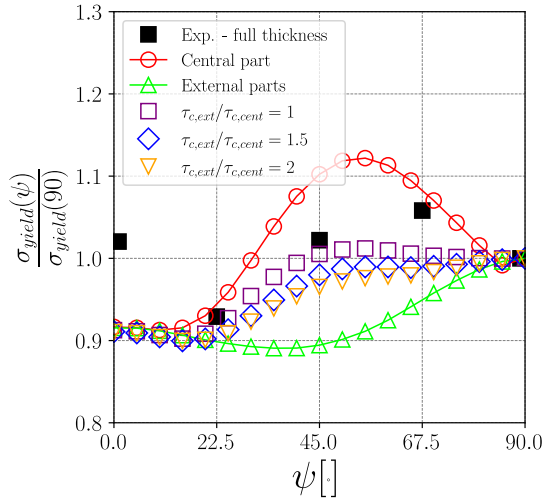


(b)

Figure 3.15: Planar anisotropy of (a) the Lankford coefficients ($R\psi$) and (b) the flow stress ratio $\frac{\sigma_{yield}(\psi)}{\sigma_{yield}(90^\circ)}$ at $\varepsilon_{xx} = 0.095$ as a function of the tensile axis direction ψ relative to the extrusion direction, for different volume fractions of the external parts.



(a)



(b)

Figure 3.16: Evolution of (a) Lankford coefficients (R/ψ) and (b) the normalized tensile at $\epsilon_{xx} = 0.095$ as a function of the tensile axis direction ψ relative to the extrusion direction, for different critical resolved shear stresses (τ_c) between internal and external regions.

3.4.3 Emergence of internal stresses after post-processing

3.4.3.1 Assessment of internal stress build-up

Figure 3.13 shows that at $\psi = 0^\circ$, 45° , and 90° , Δq values of different magnitudes and signs are predicted. These loading directions were therefore selected to examine both the magnitude and the nature of the internal stresses that develop during post-processing (here uniaxial loading).

Figure 3.17a. presents the internal stresses in the tensile direction within the external layers as predicted by the three CP models, together with the experimental measurements. The experimental data exhibited a standard deviation larger than the mean values, indicating that no statistically significant internal stresses developed in this direction for any ψ . This observation was consistently predicted by all three models, which predicted small internal stresses. For all directions, the mean-field models predicted stresses of ~ 10 MPa, whereas the CPFEM simulations predicted values < 5 MPa. No specific orientation exhibited a larger stress build-up than the others.

A higher level of internal stress was observed in the direction perpendicular to the tensile axis, as seen in Figure 3.17b.. Experimental measurements indicated significant internal stresses, with the maximum occurring at $\psi = 45^\circ$, where tensile residual stresses reached approximately 65 MPa. The crystal plasticity (CP) models also predicted the largest residual stress at $\psi = 45^\circ$, although the predicted magnitude was underestimated by approximately 35 MPa. For the other two orientations, the models predicted compressive stresses in the external layers, whereas tensile stresses were measured experimentally.

In CPFEM simulations, removing the constraint that maintained flat lateral surfaces during unloading allowed stresses to relax, leading to transverse deformation of the cross section in regions of highest internal stress. Figure 3.18 shows the corresponding stress distributions along the tensile (x) and transverse (y) directions after such relaxation. Internal stresses were no longer uniform through the layer and gradually decreased toward the free surfaces, reflecting the induced shape change. Despite this redistribution, the stress magnitude within each layer remained of the same order. In the tensile direction, the predicted average stresses in the external layers were relatively low: -3.2 MPa at 0° , -1.7 MPa at 45° , and 0 MPa at 90° . In contrast, transverse stresses remained important, with approximately 22 MPa in tension at 45° , -17 MPa in compression at 90° , and around -6 MPa at 0° .

The deformed cross-sections are shown in Figure 3.19, where barreling phenomena are clearly visible. Barreling was also observed in the experimental specimens. At $\psi = 0^\circ$, the lateral surface remained nearly flat, whereas a

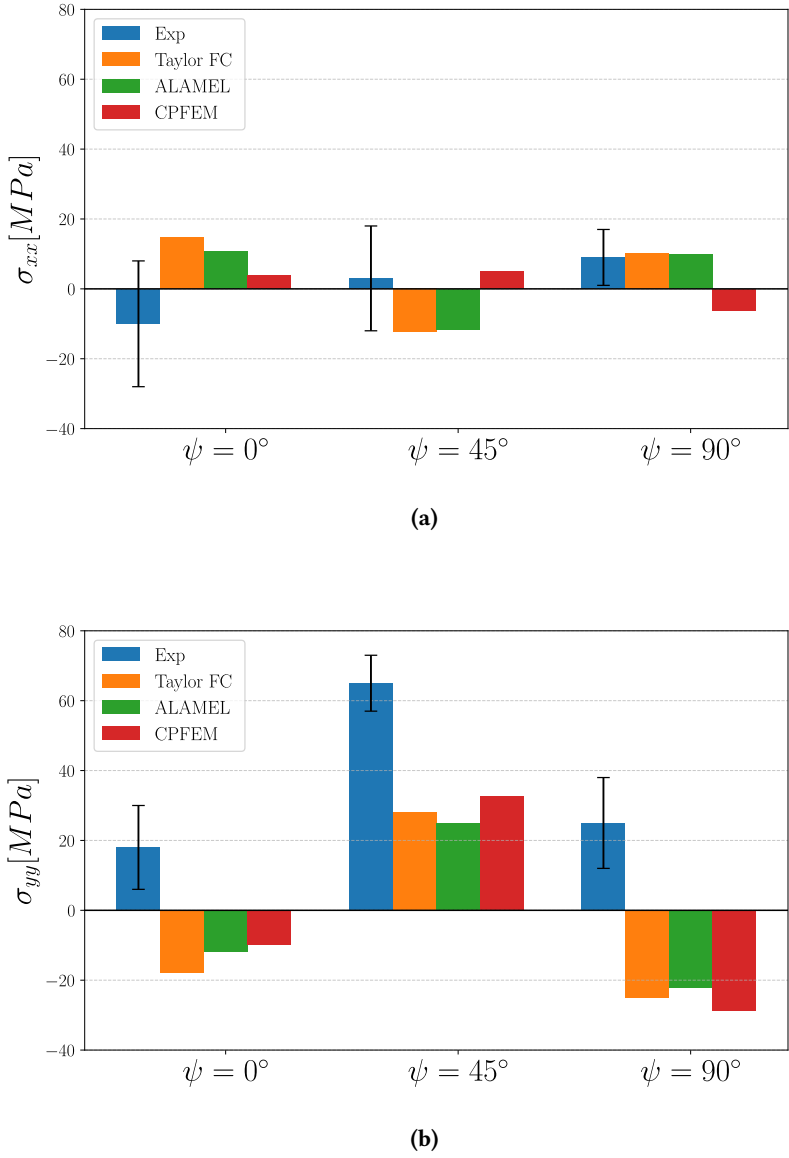
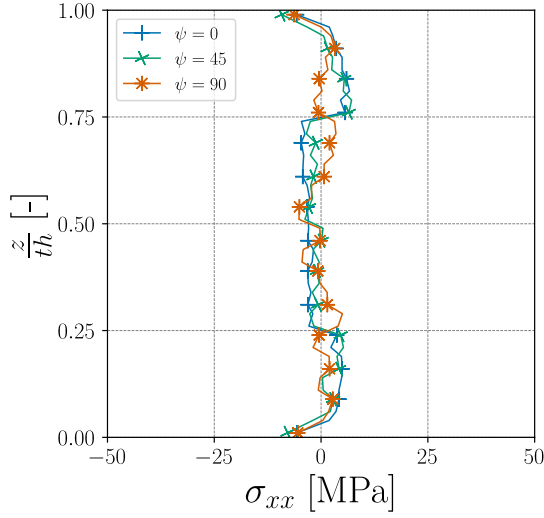
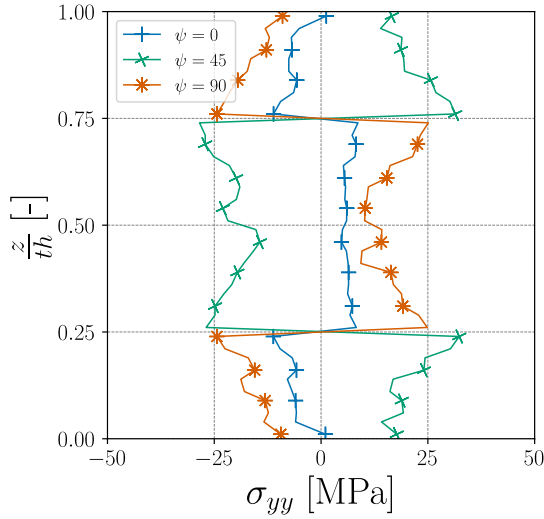


Figure 3.17: Internal stresses measured experimentally and predicted by crystal plasticity (CP) models. Internal stresses are presented for the external layers only, as CP models predict uniform stresses within each layer (the internal layer exhibits the same magnitude with opposite sign). (a) Internal stresses in the tensile direction (x) and (b) internal stresses in the transverse direction (y) are shown as a function of tensile direction ψ relative to the extrusion direction.



(a)



(b)

Figure 3.18: CPFEM predictions of the through-thickness distribution of internal stresses after removal of the flat-surface constraint. Internal stresses are shown in (a) the tensile direction and (b) the transverse direction for different tensile orientations ψ .

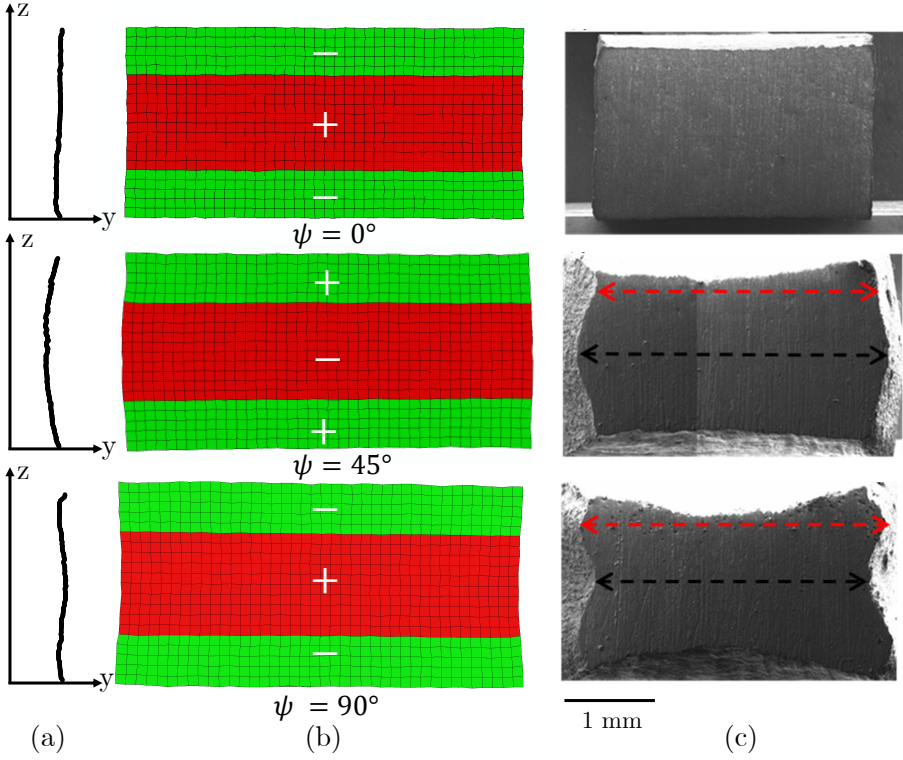


Figure 3.19: Cross-sectional profiles illustrating barreling after tensile deformation in the X-direction. (a) Profile of the vertical face measured experimentally. (b) CPFEM prediction of the deformed shape after unloading, with “+” and “-” symbols indicating regions in tension and compression. (c) Cross-sectional shape of an extruded aluminium alloy with similar microstructure and texture to AA6063 after plastic deformation (Chen et al., 2018).

concave profile developed at $\psi = 45^\circ$ and a convex profile at $\psi = 90^\circ$. CPFEM simulations reproduced the experimentally measured final section shapes and was in agreement with previously reported deformed sections of plastically deformed extruded aluminum sheets (Chen et al., 2018). It is interesting to note that the convex shape observed experimentally at $\psi = 90^\circ$ corresponds to compressive stresses in the external layers, whereas tensile stresses were deduced from X-ray diffraction in the same region. Similarly, at $\psi = 0^\circ$, the cross section was less deformed but still exhibited a concave profile, consistent with literature reports, while tensile stresses were observed experimentally in the external layers.

3.4.3.2 Bending radius due to the asymmetric relaxation of residual stresses

The presence of internal stresses can also be deduced from the curvature when one side of the plate is ground (Detor et al., 2009; Bouaouina et al., 2018; Besnard et al., 2019). This approach relies on measuring the curvature radius that develops as a result of bending. It is commonly used in the context of thin and thick films as coatings to quantify the level of internal stresses. In this section, we looked at a similar approach to reveal and quantify the internal stresses present in our specimens.

As shown previously, plastic deformation incompatibility generated substantial internal stresses in the perpendicular direction to the loading direction (y -direction). As illustrated in Figure 3.20, this stress distribution is symmetric with respect to the mid-plane and therefore satisfies the equilibrium conditions (Doghri, 2013):

$$N = \int_S \sigma \cdot e_y dS = 0 \quad M = \int_S (ye_y + ze_z) \times (\sigma \cdot e_y) dS = 0 \quad (3.1)$$

Where e_y is the unit vector along the y -direction, σ is the local stress tensor, S is the cross-sectional surface, N is the resultant stress vector, and M is the resultant moment.

Removing material from the surface disrupts this equilibrium, such that $N \neq 0$ and $M \neq 0$, forcing the sheet by a partial springback to restore equilibrium. Given the initial stress state, with some layers in tension and others in compression, the material develops a bending curvature.

Based on classical beam theory, a straight beam with a uniform cross-section subjected to a bending moment M develops a uniform curvature radius R , as illustrated in Figure 3.20. The associated strain distribution in the y -direction across the thickness is expressed as:

$$\epsilon_{yy} = \frac{z}{R}, \quad (3.2)$$

With z denotes the distance from the neutral axis to a given position through the thickness.

Therefore, if stress relaxation following material removal induces the emergence of curvature, the resulting profile of strain increment $\Delta\epsilon_{yy}$ through the thickness can be approximated as:

$$\Delta\epsilon_{yy} \simeq \frac{(z - th_{ext})}{R} \quad (3.3)$$

Here, th_{ext} is the thickness of an external layer.

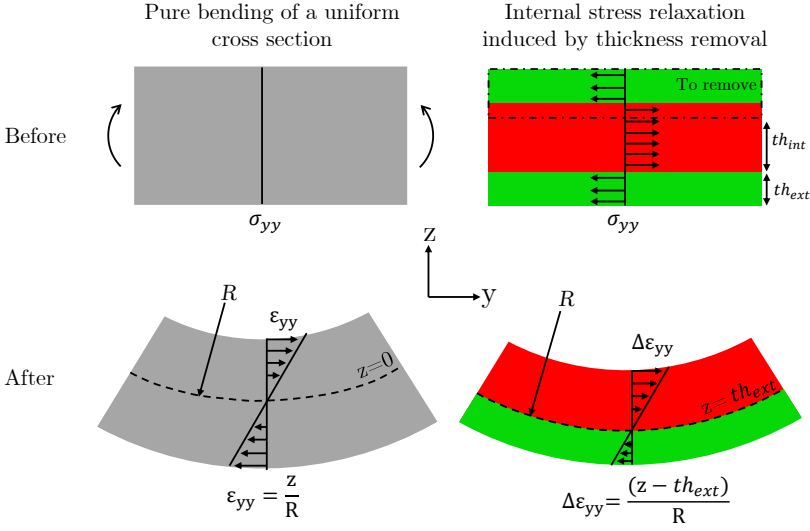


Figure 3.20: Schematic of strain distribution across the thickness induced by curvature.

Using CPFEM, the through-thickness strain increment profiles were analysed for three thinning ratios, considering that at least one of the external layers was completely removed: $\frac{th_{int}}{th_{ext}} = 2, 1.2,$ and 0.3 , where th_{int} and th_{ext} denote the remaining internal and external thicknesses after polishing. Figure 3.21 shows the averaged strain increment profiles for $\psi = 45^\circ$, obtained by averaging all integration points initially located at the same z -position. When the thinning ratio was the smallest, $\frac{th_{int}}{th_{ext}} = 0.4$, the strain increment profiles resulting from stress relaxation closely approached the theoretical linear distribution expected for pure bending of a curved beam. In contrast, for larger thinning ratios, noticeable deviations from linearity were observed due to the barreling phenomenon occurring in the thicker (central) layer. Consequently, for all loading directions investigated, a thinning ratio of $\frac{th_{int}}{th_{ext}} = 0.4$ was required to obtain a strain profile representative of pure bending. Linear regression was then applied to estimate the slope of the $\Delta\epsilon_{yy}$ profiles using all integration points of the mesh. The predicted curvature radii are reported in Table 3.10. At $\psi = 0^\circ$ and 90° , the radii were positive, whereas at $\psi = 45^\circ$ it was negative, indicating an opposite bending direction. In absolute values, the radii at $\psi = 45^\circ$ and 90° were smaller than that at 0° , confirming stronger residual stresses after tensile stress in these directions.

This approach was also tested experimentally. However, curvature measurements could not be reliably obtained due to the narrow width of the

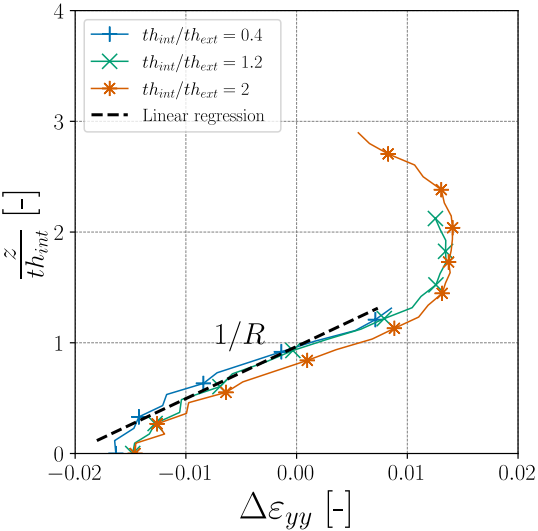


Figure 3.21: Predicted through-thickness strain increment profiles for $\psi = 45^\circ$ obtained for different thinning ratios. Strain increment $\Delta\varepsilon_{yy}$ were averaged over integration points initially located at the same z -position. The linear slope of the profiles enables determination of the corresponding curvature radius.

Curvature Radius	$\psi = 0^\circ$	$\psi = 45^\circ$	$\psi = 90^\circ$
$\frac{th_{int}}{th_{ext}} = 0.4$	-85 [mm]	28 [mm]	-26 [mm]

Table 3.10: Predicted curvature radius after thickness removal. Results are presented for various tensile direction ψ . Radii are expressed in mm. Positive and negative values indicate bending directions.

specimens (5 mm), which hindered accurate determination of the curvature radius over such small segments. Indeed, it was not possible to distinguish whether the observed non-planarity after polishing originated from curvature or from non-uniformities introduced during the electro-polishing step.

3.5 Discussion

The present analysis has investigated the plastic anisotropy arising from through-thickness texture heterogeneity and examined the link with the development of internal stresses. By combining experimental measurements with crystal plasticity (CP) simulations, the study has provided a detailed assessment of the role played by texture in governing both the macroscopic anisotropic response and the emergence of internal stresses.

The three crystal plasticity (CP) models used in this study successfully captured both the macroscopic planar anisotropy and the layer-specific anisotropy of the extruded aluminium sheet. The experimental results showed the distribution of macroscopic Lankford coefficient and flow-stress ratio as a function of the tensile direction ψ , in agreement with previously reported results for extruded aluminium alloys (Ghosh et al., 2015; Khadyko et al., 2017). When using the average texture, all three models reproduced the same Lankford curve and the same flow stress curve. Similarly, the models accurately predicted the Lankford curve corresponding to the texture of the central layer, consistent with earlier studies (Li et al., 2005; Chen et al., 2018). Predictions based on the peripheral texture indicated lower Lankford coefficients at 0° and 90° compared to the central layer. While no experimental data directly confirm this trend, previous simulations using a VPSC approach with both central and peripheral textures reported a similar relative behavior (Chen et al., 2018). Additional evidence for the consistency of the model predictions for the outer layer is provided by the observation that the Lankford curves for the central and peripheral layers intersect near 15° and 67.5° , which corresponds closely to the experimentally measured macroscopic Lankford coefficient along these loading directions. These results demonstrate that the models effectively capture the plastic anisotropy behaviour of both layers and support the hypothesis that texture is the primary source of plastic anisotropy in such aluminium (Oscarsson et al., 1991; Bate and An, 2004; Engler and Aegerter, 2014). The flow stress anisotropy was not so well predicted close to the extrusion direction. The models predicted a σ_{yield} mostly constant and close to $0.9\sigma_{yield}(90^\circ)$, whereas the experiments provided $\sigma_{yield}(0^\circ) > \sigma_{yield}(90^\circ)$ and $\sigma_{yield}(0^\circ < \psi \leq 25^\circ) < \sigma_{yield}(0^\circ)$. These experimental features were captured by neither average nor layer-specific texture simulations. Furthermore, the evolution of the Taylor factor in the core material, which increases only

slightly between 0° and 22.5° , is insufficient to explain the measured yield stress variations. The observed deviation between the experimental data and the numerical predictions could be partially attributed to the formation of Guinier-Preston (GP) zones, which are nanoscale solute clusters precipitated during natural aging (Esmacili and Lloyd, 2004; Yin et al., 2016). The influence of such precipitates on plastic anisotropy was highlighted by Kuwabara et al. (2017), who investigated the anisotropic response of textured AA6061 in both O and T4 tempers and noted that the directional dependency in the plastic response presumably depends on GP zones as well as crystallographic texture. Furthermore, Khadyko et al. (2017) reported variations in the flow stress of AA6063 between the 0° and 22.5° loading directions when comparing O and T1 tempers. The authors mentioned that these variations, which align well with the observations in the present study, could be possibly the result of GP zones. In the current work, the extruded sheets were stored at room temperature for approximately two years prior to testing. Consequently, it is probable that the alloy underwent natural aging, inducing formation of GP zones; however, no experimental characterization were made to confirm this. Because the employed crystal plasticity models do not account for these precipitates, they may inherently underestimate the yield stress along certain crystallographic directions.

As widely reported in the literature, using the average texture provides reliable predictions of the anisotropic behaviour for such extruded aluminium sheet (Bate and An, 2004; Engler and An, 2005; Ghosh et al., 2015; Khadyko et al., 2016, 2017). Closer agreement with the experimental Lankford curve can be obtained by assigning a slightly greater contribution to the plastic response of the outer layer. It can be achieved either by assuming a thicker peripheral layer, since the layer boundaries are not clearly defined, or by artificially increasing its hardness, which could be justified by its smaller grain size. However, the latter hypothesis is inconsistent with microhardness measurements, which indicate no significant variation through the sheet thickness.

Considering the strong hypotheses made, the three CP models provided satisfactory predictions of the internal stresses when compared with the experimental observations. Residual stresses measured on the external surfaces indicated negligible internal stresses along the tensile (X) direction for all direction ψ relative to the extrusion direction, whereas significant stresses developed in the transverse (Y) direction. The three models reproduced these trends. An additional qualitative indicator of internal-stress magnitude is the degree of cross-sectional distortion caused by barreling. Experimentally, only minor distortion was observed at $\psi = 0^\circ$, whereas a highly heterogeneous cross-section deformation occurred at $\psi = 45^\circ$ and 90° . This behavior conforms to the predicted internal stress magnitudes in Y -direction, which showed

considerably larger absolute values after tension at 45° and 90° compared to 0° relative to the extrusion direction, further confirming the consistency between model predictions and experimental observations. The main discrepancy between predictions and measurements concerns the internal stresses probed by X-ray diffraction in the external layers at $\psi = 0^\circ$ and 90° . Experimentally, tensile residual stresses were measured after all tensile tests, whereas the models predicted compressive stresses at 0° and 90° . However, the cross-sectional distortion measured at these orientations indicates that the external layers should be in compression, suggesting that the discrepancy arises from inaccurate X-ray measurements issues at $\psi = 0^\circ$ and 90° rather than from the models. This experimental deviation could be due to the limitations of the Debye-Scherrer method when applied to the coarse-grained microstructures present on the surface (PCG). The method relies on the statistical assumption that the irradiated volume contains a sufficient number of grains to generate continuous, ideal diffraction rings. In the present case, the coarse grain size gives discontinuous diffraction patterns. Consequently, the measured values likely reflect local intergranular stresses of individual crystallites rather than the representative macroscopic average stress.

Comparing the predicted q -values of the different layers also made it possible to identify the loading directions most likely to generate significant internal stresses, as well as their qualitative distribution (compression or traction stress state). Indeed, the q -values predicted by all three models indicate that, for orientations below 15° and above 67.5° , the central layer contracts more in the transverse direction than the outer layer. This discrepancy is expected to induce tensile stresses in the central layer and compressive stresses in the outer layer. The opposite behaviour occurs between 15° and 67.5° , where the outer layer exhibit higher q -values. The largest differences in q -values are predicted at $\psi = 45^\circ$, corresponding to stronger strain incompatibilities and, consequently, larger residual stresses. The information obtained from this simple comparison of q -values are consistent not only with the predicted distribution of internal stresses but also with their relative magnitudes when both textures are accounted for within the same simulation. To further demonstrate the potential of this approach, the same methodology was applied to assess the development of internal stresses in a roll-bonded multilayer composed of alternating 316L and AISI 410 stainless steel layers. Comparison of the q -values distributions associated with the experimentally measured textures suggests an even larger discrepancy in plastic behaviour than that observed in the extruded sheet studied here. Further details are provided in Appendix B.

Based on these analyses, it can be concluded that all three crystal plasticity models successfully captured the plastic anisotropy of the extruded aluminium sheet and accurately predicted both the magnitude and orientation of internal

stresses arising from through-thickness texture heterogeneity. None of the models clearly outperformed the others, as their predictions were very similar. This similarity may be attributed to the dominance of a single, strong texture component (Cube {001}<100>), which reduces the influence of grain–grain interactions and thereby limits the benefits typically offered by more advanced formulations, such as ALAMEL or CPFEM. However, further investigation would be required to confirm this hypothesis. These observations suggest that mean-field approaches are well suited for estimating plastic anisotropy and internal stress development in such extruded sheets, as they provide accuracy comparable to CPFEM while requiring substantially less computational effort. The use of CPFEM is only necessary to capture the barrelling phenomenon associated with stress relaxation.

3.6 Conclusion

Extrusion of AA6063 sheets is often accompanied by a heterogeneous distribution of texture through the thickness, with a clear difference between near-surface and bulk. This study demonstrated the different plastic anisotropy associated with these two textures differed can give rise to significant residual stresses across the sheet thickness after post-processing of the extruded sample. The main findings can be summarized as follows:

- Comparison between predictions and experimental measures confirms that the internal stresses arise from the incompatibility between the anisotropic plastic responses of the surface and central regions, which in turn originates from their distinct textures. When layer-specific textures are taken into account, the crystal plasticity models predict both the magnitude and the through-thickness distribution of the internal stresses in good agreement with experimental observations.
- The loading directions most likely to promote significant internal stress development, as well as the sign and through-thickness distribution of these stresses, can be readily identified by comparing the distributions of q -values distributions associated with the different textures for various loading directions
- Predictions indicated that macroscopic plastic anisotropy results from a balance between the different responses of the surface and the central layers. For the loading directions at 15° and 67.5° with respect to the extrusion direction, the layers exhibit similar anisotropic responses, suggesting that no internal stresses develop for these loading orientations.

- The three CP models employed in this study (Taylor FC, ALAMEL and CPFEM) made similar predictions. Whether using the through-thickness average texture or the textures of the layers, all models accurately reproduced the measured plastic anisotropy. They also captured both the magnitude and orientation of the internal stresses observed experimentally in each layer. Given that the mean-field models achieved this accuracy at substantially lower computational cost than CPFEM, they represent an efficient and reliable choice for analysing plastic anisotropy and assessing the development of internal stresses in extruded AA6063 sheets.

Strain and texture heterogeneity across roll-bonded metal sheets

4

The geometry of the tools in a manufacturing process may strongly influence the development of crystallographic texture. Several forming processes produce distinct textures, which have been extensively characterized in the past due to their significant impact on the anisotropic behaviour of the final product. In processes such as extrusion or rolling, the strain paths are not uniform across the thickness, leading to gradients in the accumulated plastic deformation and the residual stresses. In this chapter, we explore the possibility of using texture as an indicator of the heterogeneity of the plastic strain field induced by the process. In particular, we focus on the texture gradients generated during roll-bonding within a multi-laminate.

The chapter is organized as follows. The introduction reviews the current understanding of the relationship between strain and texture development during rolling. The material and experimental procedures used to produce the studied multi-laminates are presented in Section 4.2. Section 4.3 details the numerical framework proposed to link plastic deformation with the associated texture evolution. This framework is then validated against literature results for single- and multi-pass rolling in Section 4.4. The analysis of the deformation field and the corresponding texture in two different multi-laminates is presented in Section 4.5. Finally, the results are discussed in Section 4.6, followed by the conclusions.

Some of the work included in this chapter has been published:

- **Hanon, G.**, Malet, L., Delannay, L., Texture and Microstructure After Roll-Bonding of an Fe-Al Multilaminate, Proceedings of the 14th International Conference on the Technology of Plasticity, 2023.
https://doi.org/10.1007/978-3-031-40920-2_67
- **Hanon, G.**, Malet, L., Delannay, L., Heterogeneity of strain and texture inside roll-bonded multilaminates, Materials Research Proceedings, 2024.
<https://doi.org/10.21741/9781644903131-191>

4.1 Introduction

Roll bonding of metallic sheets with contrasted mechanical properties may result in high-performance layered composites (Dehsorkhi et al., 2011; Wang and Misra, 2011; Chang et al., 2012; Mashhadi et al., 2017). The roll-bonding process typically requires a large reduction ($\sim 50\%$) of the sheet thicknesses in a single rolling pass, thus involving significant microstructural changes. Due to the mismatch of strength, achieving co-deformation of the assembly is much more challenging with the risk that the harder phase tends to fragment with the emergence of inclined shear bands inside the softer phase (Govindaraj et al., 2013; McCabe et al., 2021). This undesirable result should be avoided or limited as it hinders achieving composite mechanical properties and is hence likely to reduce ductility, strength and toughness. Ensuring the most uniform possible deformation across all layers is therefore essential. In this context, a quantitative evaluation of the through-thickness strain heterogeneity is essential to guide process optimization.

Even in single-phase metallic sheets, cold rolling inherently induces a heterogeneous plastic strain distribution through the thickness, driven by non-uniform shear deformation. Two main factors are identified to influence this heterogeneity: the friction at the roll-sheet interface and the roll-gap geometry (Yang et al., 2010). The latter, also named rolling draught, is commonly expressed l_c/th , where l_c is the contact length and th the mean sheet thickness ($th = \frac{th_{in} + th_{out}}{2}$). Small draught configuration correspond to $l_c/th < 0.5$, intermediate configuration to $0.5 < l_c/th < 5$ and large draught to $l_c/th > 5$. Although, material parameters such as yield strength and hardening exponent may also affect the strain distribution (Truszkowski et al., 1982; Major, 1992), their influence is secondary compared with friction and rolling draught. Due to the symmetry of the rolling process, the shear strain always vanishes at the mid-thickness.

Direct experimental measurement of the through-thickness plastic deformation in rolled multilayers remains not straightforward. Several approaches have been developed to estimate the local deformation gradient. Through-thickness lines of microhardness indents on a side free surface can be used to track relative displacements and extract plastic strain based on the evolution of the indent shapes and their relative positions after rolling (Roumina and Sinclair, 2008). Embedded pins offer another means to reconstruct the deformation field by comparing their final shapes with numerical predictions (Das et al., 2001; Li et al., 2010). Inserts engraved with a reference grid provide another approach to measure the plastic strain after rolling based on the deformation of the grid (Boldetti et al., 2005). Digital Image Correlation

(DIC) techniques have also been implemented for in-situ monitoring of strain fields during rolling (Li et al., 2003). More recently, a novel approach called Time-Integrated Digital Image Correlation (iDIC) method has exploited the steady-state character of the process to improve accuracy and robustness (Hoefnagels et al., 2022; Jacobs et al., 2022). Simpler qualitative approaches, such as vertical scratch lines through the thickness, provide only local and final-state information (Tamimi et al., 2014).

In contrast, through-thickness crystallographic texture can be measured without any pre-processing of the sample and can probe the bulk. In the absence of shear, texture presenting an orthorhombic symmetry develops at mid-thickness. In FCC metals, the central region typically exhibits a pronounced β -fibre, characterized by strong Copper $\{112\}\langle 111\rangle$, S $\{123\}\langle 634\rangle$ and Brass $\{110\}\langle 112\rangle$ components, displaying an orthorhombic symmetry (Choi et al., 1997). Increasing strain further strengthens this fibre, although the evolution of the individual components differs: Copper and S components intensify, while the Brass component weakens (Mishin et al., 2010). In BCC metals, both the α - and γ -fibres strengthen with increasing reduction. However, for reductions over 80%, the α -fibre becomes dominant while the γ -fibre progressively depletes (Hölscher et al., 1991; Ray et al., 1994; Ashby et al., 1999). When shear is introduced through friction at the roll-sheet interface, the resulting texture rotates about the transverse direction, gradually shifting from the conventional rolling fibres toward the ideal shear-deformation components. In FCC metals, grain orientations initially associated with the β -fibre progressively rotate toward the characteristic shear components $\{001\}\langle 011\rangle$, $\{111\}\langle 112\rangle$, and $\{111\}\langle 110\rangle$ as the imposed shear increases (Kim and Lee, 2001; Sakai et al., 2001). This texture disrupts the characteristic orthorhombic symmetry associated with pure plane-strain compression (Choi et al., 1997).

In single-phase metallic sheets, texture gradients are intrinsically linked with strain gradients and are strongly influenced by friction conditions and rolling draught. Under small draught conditions ($l_c/th < 0.5$), shear textures were shown to develop primarily near the quarter-thickness positions, whereas under large draught ($l_c/th > 5$), shear components dominated near the sheet surface (Truszkowski et al., 1980). Intermediate draught conditions generally lead to more homogeneous textures across the thickness. For example, a 40% thickness reduction of AA1050 at $l_c/th = 1.92$ exhibited a nearly uniform texture profile through the thickness (Mishin et al., 2000). It was shown that lubrication conditions also played a significant role: high friction coefficient enhanced deviations from the orthorhombic rolling texture (Huh et al., 1999; Kang et al., 2007; Chen et al., 2011) and promoted deeper penetration of shear deformation (Choi et al., 1997).

Determining the local plastic strain state based only on the final texture is not straightforward and generally requires numerical simulations. In rolling, this was commonly done in two steps. First, the through-thickness deformation gradients were predicted using macroscopic finite element models simulating the rolling pass, assuming isotropic elasticity and J2 plasticity (Choi et al., 1997; Kang et al., 2007; Li et al., 2010; Yang et al., 2010). The deformation gradients extracted from the FE simulations were then used to predict the corresponding texture evolution using crystal plasticity models such as Taylor FC (Lee and Duggan, 1991; Aukrust et al., 1997; Delannay and Mishin, 2013), Taylor RC (Aukrust et al., 1997; Pérocheau and Driver, 2000), ALAMEL (Li et al., 2010; Delannay and Mishin, 2013; Shore et al., 2018), GIA (Engler et al., 2005; Cantergiani et al., 2024) and VPSC (Engler et al., 2000; Tamimi et al., 2014). A fully integrated (all-in-one) approach was also used to simulate the rolling pass directly using Crystal Plasticity Finite Element Models (CPFEM), although this method was computationally much more demanding (Schoenfeld and Asaro, 1996; Si et al., 2008; Deng et al., 2014).

In multilayers produced by roll bonding, additional strain heterogeneity is expected due to the strength contrast of the successive layers. The parameters (rolling draught and friction condition) inducing strain heterogeneity in single-phase sheets are likely to remain operative. This work aims to address the following questions:

- What is the through-thickness strain heterogeneity in a multilaminate produced by roll bonding?
- Can the final crystallographic texture be used probe such heterogeneity?

4.2 Preparation and characterisation of roll-bonded samples

I carried out the preparation of the different layers, the roll-bonding process, and the preparation of samples for EBSD measurements, while all EBSD measurements were performed by Dr. Loïc Malet from Université Libre de Bruxelles (ULB).

5- and 9-layer multi-laminates were successfully roll-bonded at ambient temperature. The materials, experimental setup and procedures used for both were identical.

Two common metal grades were selected for the present work. With a yield stress of 40MPa and a UTS of 120MPa, the 1050 aluminium alloy sheets were about three times softer than the sheets made of ARMCO steel ($\sigma_{yield} = 145\text{MPa}$ and $\sigma_{UTS} = 300\text{MPa}$). Before being stacked and roll-bonded,

both metals had equiaxed grains and very weak crystallographic textures. Due to the strength contrast, it was a real challenge to prevent relative motion of the sheets at the entrance of the roll gap. Successful bonding was achieved by preliminary folding the outer sheet around one or several inner layers, thereby constraining relative motion. The successive folding steps are shown in Figure 4.1.

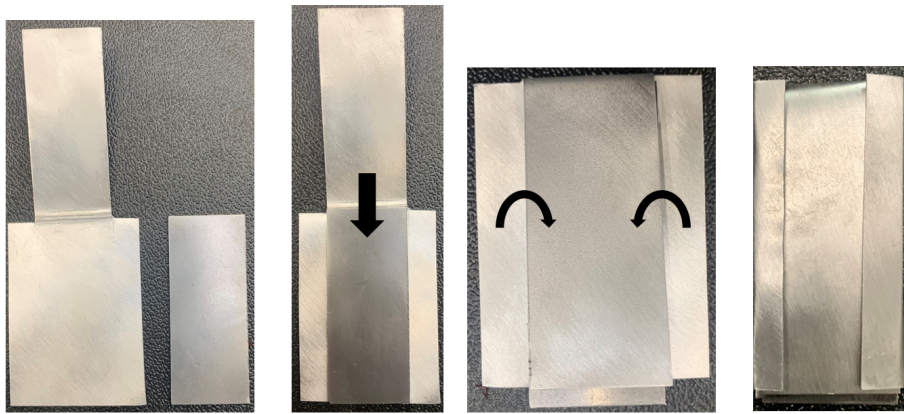


Figure 4.1: Before the first rolling pass, the aluminium sheet is folded around the iron sheet to prevent relative motion. The latter would impede bonding.

Different roll-bonding routes were used to produce the 5-layer and 9-layer multilaminates.

For the 5-layer multi-laminate, roll-bonding was achieved in two steps. The first rolling pass was applied to a stacking of two 0.4mm-thick AA1050 sheets separated by a single 0.8mm-thick iron sheet. The total thickness was reduced to 0.62mm, which corresponds to 61% thickness reduction. Between the two rolling passes, the 3-layer composite was held at 500°C during 30 minutes, which allowed annealing the AA1050 sheet. Then, two 0.2mm-thick iron layers were added on either side of the 3-layer composite sheet. The second rolling pass reduced the total thickness to 0.62mm, which corresponds to an extra 39% thickness reduction.

Two rolling passes were also required to obtain the 9-layer stack. To start, a 3-layer was obtained by rolling a 0.8 mm-thick Iron sheet wrapped inside a 0.4 aluminium sheet folded in two. The first rolling pass involved 61% thickness reduction to ensure bonding. Two such three-layer units were produced and subsequently heat treated at 500 °C for 30 min. For the second pass, the two units were stacked symmetrically with a central 0.2mm Fe layer and wrapped inside a 0.2 mm thick Fe sheet. The second rolling pass applied a 62% thickness reduction.

All to-be-bonded surfaces were preliminary degreased in Acetone and brushed with a 0.3 mm diameter wire-brush in order to remove any oxide layer. Rolling was performed on a laboratory cold-rolling mill having a rolls diameter of 112mm and no lubrication was used during processing. The complete processing routes for the 5-layer and 9-layer laminates are summarised in Figures 4.2a and 4.2b.

The crystallographic texture was probed within each layer of both multi-laminates using electron back scatter diffraction (EBSD). This required prior polishing using SiC up to grid 1200 followed by diamond suspension up to 1 micron and OPS. The orientation maps were colored according to the inverse pole figure (IPF) relative to the rolling direction (RD). For the 5-layer specimen, an EBSD map was acquired over a $176.7 \mu\text{m} \times 353.3 \mu\text{m}$ region using a step size of $0.3 \mu\text{m}$, yielding 751070 data points. To resolve finer microstructural details within the aluminium layer, a high-resolution scan was subsequently conducted over a localized $17.7 \mu\text{m} \times 17.7 \mu\text{m}$ area with a reduced step size of $0.05 \mu\text{m}$ (126025 data points). For the 9-layer specimen, four distinct EBSD maps were collected. Each scan covered an area of $492 \mu\text{m} \times 490.5 \mu\text{m}$ using a step size of $1.5 \mu\text{m}$, resulting in a cumulative total of 431888 data points across the analysed regions.

In the 5-layer multi-laminate, optical microscopy observation of the sheet longitudinal cross-section (Figure 4.3) confirmed balanced co-deformation of the two metals and uniform thickness reduction in all layers. A thin oxide film at the interface (not fully eliminated after the inter-pass heating) did not impede successful bonding. The iron layer located at the sheet mid-thickness (left on Figure 4.3) had elongated grains and a typical texture of cold rolling. The pole figure of the external layer made of iron does not show a clear texture. This layer was added after the first rolling pass and it was hence less deformed than the central layers. The aluminium layer showed a refined equiaxed microstructure. Based on the high indexation rate in the close-up EBSD scan, we suspected continuous recrystallization.

Figure 4.4 shows a section of the 9-layer multi-laminate produced. Grey contrast in the optical microscope clearly identifies the 9 layers made of the two different metals. Four different zones were measured by EBSD, each one covering the plate thickness. One such orientation maps is shown in Figure 4.4 (blue square). Flat and elongated grains were found in all Fe layers whereas Al layers hosted a very refined equiaxed microstructure. The $\{111\}$ pole figures shown in Figure 4.4 are representative of individual layers. They were produced by combining suitable zones in the four orientation maps. Note that only the 7 central layers are represented. The peripheral layers were excluded due to weak texture and poor indexing, defined here as low confidence in automated orientation determination resulting from degraded Kikuchi pattern quality.

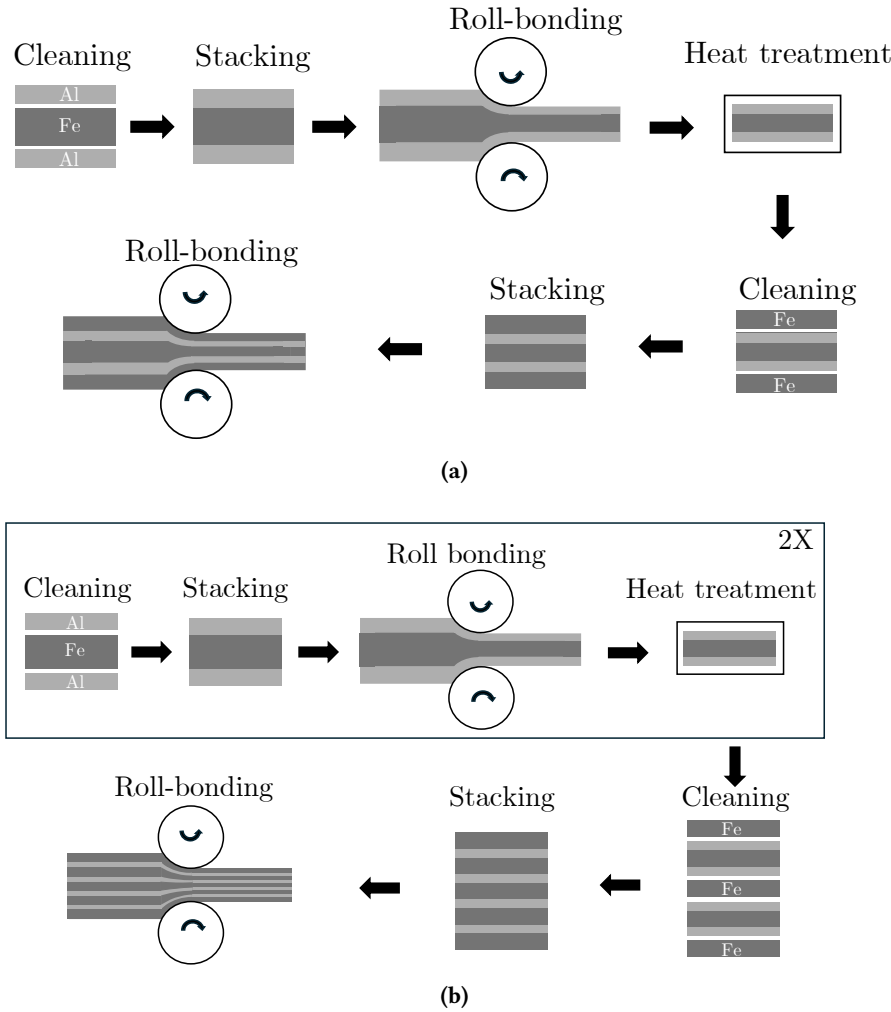


Figure 4.2: Schematic of the experimental procedure used for roll-bonding the Fe–Al multilayer composed of (a) 5 and (b) 9 stacked layers.

For both multi-laminates, crystallographic texture analysis was performed using the MTEX toolbox (Hielscher and Schaeben, 2008). The Orientation Distribution Function (ODF) was reconstructed from discrete EBSD measurements via Kernel Density Estimation (KDE). This estimation employed a radially symmetric de la Vallée Poussin kernel with a constant half-width of 10° . The numerical computation was executed using the spectral method based on Generalized Spherical Harmonics, which optimizes the convolution efficiency for large datasets. Texture visualization was performed through ODF sections and pole figures using a stereographic projection.

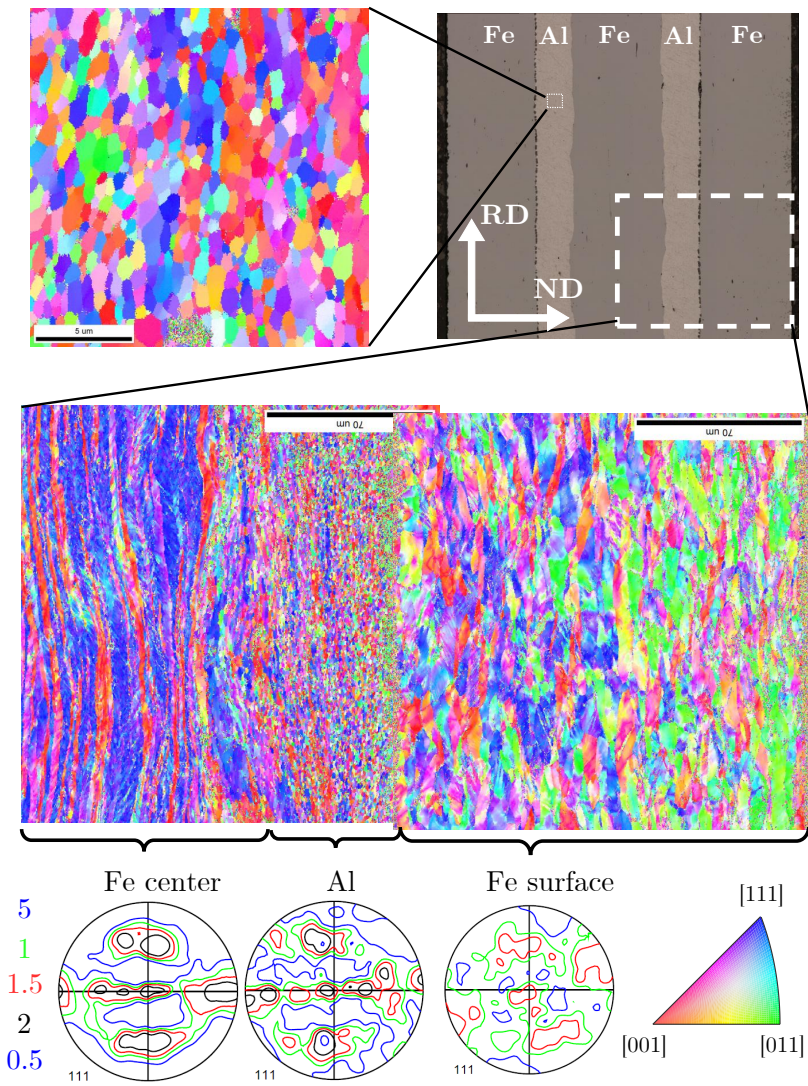


Figure 4.3: Microstructural characterization based on optical microscopy and EBSD. The coloring of orientation maps is according to the RD-IPF. The $\{111\}$ pole figures show the textures developed in the Fe and AA1050 layers.

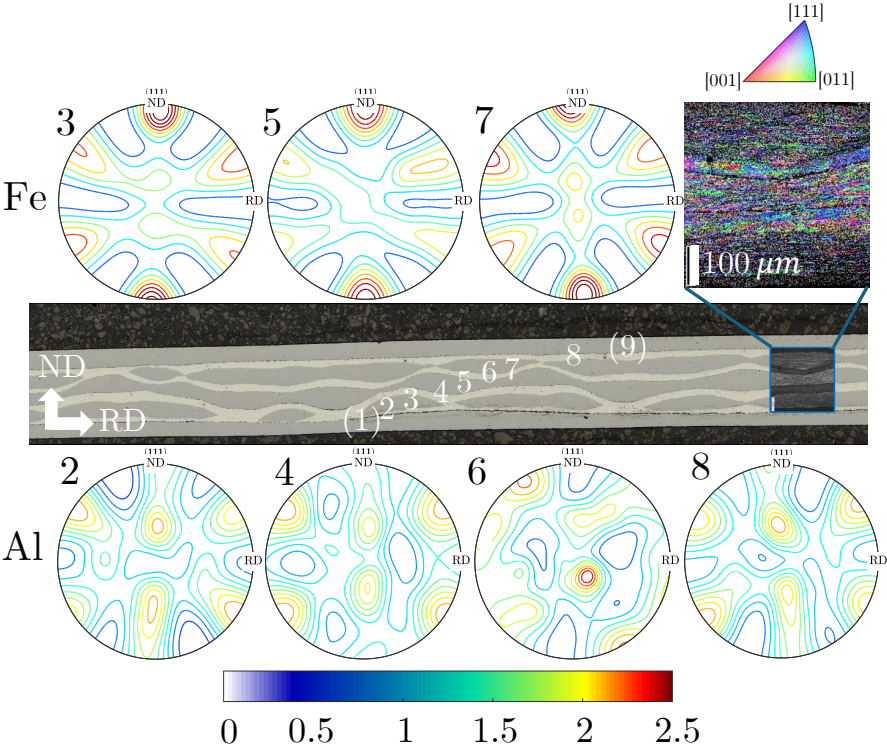


Figure 4.4: Characterization of texture and microstructure based on EBSD and optical microscopy. $\{111\}$ Pole figures (numbered according to the position in the stacking) present the texture developed inside each layer in with the rolling direction (RD) pointing to the right and the normal direction (ND) pointing to the top.

4.3 Numerical framework for single and multi-pass rolling simulations

Understanding the relationship between plastic strain heterogeneity and the development of through-thickness texture gradients requires a numerical framework that operates consistently across macroscopic and microscopic length scales. To meet this objective while maintaining computational efficiency and modelling flexibility, the framework was divided into two hierarchically coupled models:

- A macroscopic finite element (FE) model used to simulate the rolling pass and predict the deformation field across the thickness.
- A microscopic crystal plasticity (CP) model used to predict texture evolution from the imposed deformation path.

The two models were coupled through the deformation history. For a given normalized thickness position, $s = \frac{z}{t_{in}}$, the evolution of the deformation gradient $F(t)$ obtained from the macroscopic model was prescribed as boundary condition governing the deformation of the polycrystalline aggregate in the CP simulations. A complete description of the deformation path was essential, as a previous study had shown that the simultaneous evolution of F_{13} and F_{31} had a stronger influence on the predicted texture than their final values alone (Mishin et al., 2000).

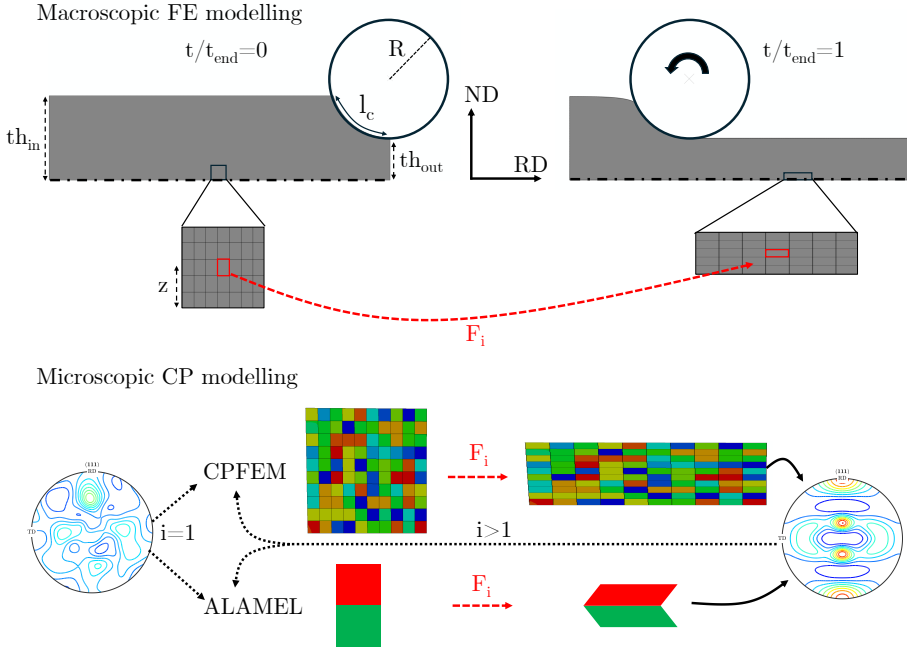


Figure 4.5: Numerical framework for simulating single-pass ($i = 1$) and multi-pass ($i > 1$) rolling. Macroscopic finite element (FE) model provides the deformation gradient field associated with each rolling pass, which is subsequently imposed as the kinematic constraint governing the deformation of the polycrystal in the microscopic crystal plasticity model. This hierarchical coupling enables the polycrystal to evolve consistently with the macroscopic deformation history across successive passes.

The macroscopic through-thickness strain field was computed using a 2D finite element model representing the deformation of a metallic sheets inside the roll gap. Plane-strain conditions were assumed, as deformation in the transverse direction was negligible in regions sufficiently far from the sheet edges due to frictional constraints at the roll-sheet interface. Exploiting the symmetry of the rolling process with respect to the mid-plane, only half of

the sheet thickness was modelled and a symmetry boundary condition was imposed along the mid-plane. The initial geometry was defined such that the leading edge of the sheet was fully in contact with the roll surface along the entire arc of contact, as illustrated in Figure 4.5. The simulation time was set sufficiently long to reach a steady-state deformation regime.

The material behaviour was described by isotropic $J2$ elasto-plasticity with a power-law hardening rule expressed as :

$$\sigma_y = \sigma_{y,0} (1 + K \varepsilon_p)^n \quad (4.1)$$

Where σ_y is the flow stress, $\sigma_{y,0}$ the initial yield stress, K and n are hardening parameters. Material constants for commercially pure aluminium and ARMCO iron were calibrated to reproduce the experimental tensile curves reported in (Li et al., 2010; Kostina et al., 2014). The calibrated parameters are listed in Table 4.1, and the resulting tensile curves are shown in Figure 4.6.

The two rolling passes performed experimentally to produce both multilaminates investigated were reproduced using the macroscopic FE model. For the first pass (common to both multilaminates) the half-thickness mesh contained 12400 plane-strain elements (CPE4). The outer half of the mesh was assigned AA1050 properties, while the inner half was assigned ARMCO iron properties. For the 5-layer multilaminate, the second pass was simulated using 31900 elements. To assess the influence of a non-uniform strength distribution on the through-thickness strain field, two variants of the second pass were performed: (i) using ARMCO iron properties for all the elements, and (ii) assigning AA1050 properties to elements belonging to the aluminium layers. For the 9-layer multilaminate, 55000 elements were used for the second pass with Armco Iron and Pure Al alloys properties distributed according to the experimental layer sequence. In all multilayer simulations, the interfaces were considered as tied from the onset of the simulation.

The rolling mill was considered to be perfectly rigid and frictional effects at the roll-sheet interface were described using Coulomb's friction law with a friction coefficient $\mu = 0.3$ which is reasonable for cold rolling process without lubrication (Li et al., 2010).

The rolling simulations were performed using an implicit dynamic analysis with direct time integration. For such analysis, Abaqus employs the Hilber-Hughes-Taylor (HHT) operator as direct-integration method by default.

Texture evolution across the sheet thickness was predicted using crystal plasticity (CP) modelling. Two CP models were employed: a crystal plasticity finite element model (CPFEM) and the mean-field model ALAMEL, the latter being selected for its ability to accurately reproduce rolling textures in aluminium alloys (Van Houtte et al., 2005). CPFEM simulations used a periodic aggregate consisting of 1000 brick-shaped grains ($10 \times 10 \times 10$), each

	E [GPa]	ν [-]	σ_y [MPa]	K [-]	n [-]
Al	69	0.3	40	1725	0.2
Fe	210	0.3	145	1448	0.13

Table 4.1: Material parameters of commercially pure aluminium and iron used in the macroscopic FE simulations.

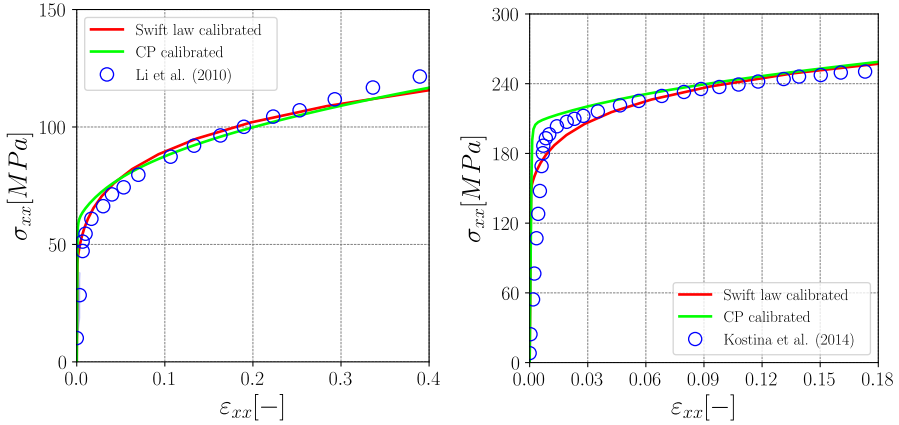


Figure 4.6: Experimental tensile curve of (a) commercially pure aluminium (Li et al., 2010) and (b) commercially pure aluminium iron (Kostina et al., 2014) compared with the simulated macroscopic and microscopic tensile curves obtained using the parameters listed in Tables 4.1 and 4.2.

Material	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	τ_{c0} [MPa]	Γ_0 [-]	n [-]	m [-]	$\dot{\gamma}_0$ [1/s]
Al	107.3	60.9	28.3	23	0.05	0.2	100	0.01
Fe	231.4	134.7	116.4	85	0.1	0.13	100	0.01

Table 4.2: Material parameters of commercially pure aluminium and iron used for the microscopic simulations.

represented by a 20-node hexahedral element (C3D20), as an accurate representation of grain morphology is not essential for texture prediction (Bronkhorst et al., 1992). Periodic boundary conditions were applied (details in Appendix F). ALAMEL simulations used the same number of grains for consistency. ALAMEL was used to investigate the texture evolution within the 5-layer multi-laminate, while CPFEM was employed for the 9-layer multi-laminate, for which more complex boundary conditions were required.

As usually assumed, the FCC phase was allowed to deform by $\{111\} \langle 110 \rangle$ dislocation glide, whereas the BCC phase allowed slip on both $\{110\} \langle 111 \rangle$ and $\{112\} \langle 111 \rangle$ systems. All simulations were initialised with random crystallographic orientations, consistent with experimental observations showing no initial texture in the metallic sheets.

Microscopic hardening parameters for both materials were calibrated to the same experimental tensile data used for the macroscopic model, while single-crystal elastic constants were taken from Hosford (1993). The resulting parameters are summarized in Table 4.2, and the corresponding tensile responses are shown in Figure 4.6.

When multiple passes are involved, simulating the complete rolling schedule in a single FE analysis is challenging due to excessive mesh distortion, which may compromise accuracy and increase computational time. Therefore, each rolling pass was simulated individually with the macroscopic FE model. For each pass, the history of the deformation gradient at selected through-thickness positions was extracted and sequentially imposed on the polycrystal to reconstruct the full deformation path. This simplification is appropriate for materials exhibiting limited work hardening, otherwise, the macroscopic constitutive parameters would need being updated between passes. Accordingly, this cumulative deformation framework was employed to predict texture evolution within the iron layers. In contrast, a different kinematic assumption was adopted for the aluminium layers, for which the deformation history associated with the first rolling pass was not considered in the texture analysis. This choice is justified by the intermediate annealing treatment applied prior to the second pass, which induces recrystallization and eliminates the crystallographic texture developed during the first rolling pass. An alternative strategy would be to use an Arbitrary Lagrangian-Eulerian (ALE) adaptive

th_{out}/th_{in}	R	l_c/th	μ
50%	18 [mm]	0.5	0.3
50%	178 [mm]	2	0.3
50%	550 [mm]	3.5	0.3
50%	1123 [mm]	5	0.25
50%	1123 [mm]	5	0.3
50%	1123 [mm]	5	0.35

Table 4.3: Summary of the different rolling simulations. The sheet thickness th used to calculate the rolling draught is defined as the mean value between inlet and outlet thicknesses: $th = \frac{th_{in} + th_{out}}{2}$.

meshing strategy to preserve mesh quality under large deformations (Boman and Ponthot, 2004). Such approach would enable all passes to be simulated in a single simulation while accounting for hardening evolution. Although not implemented in the present work, ALE could be a future improvement of the proposed framework.

Prior to analysing multilaminate heterogeneities, the framework was validated by studying the rolling of a homogeneous sheet made of commercially pure aluminium. Several rolling configurations were investigated by varying roll-gap geometry and friction coefficient. Large, intermediate, and small draughts were simulated, covering a representative range of cold-rolling conditions. The friction coefficients of 0.25, 0.30 and 0.35 were considered, consistent with typical values used in cold-rolling simulations (Choi et al., 1997; Cantergiani et al., 2024). A fixed initial sheet thickness was used and 51 elements were used across the thickness to resolve strain gradients. The main simulation parameters are summarized in Table 4.3. Texture predictions for these cases were performed using ALAMEL. Additionally, texture evolution in commercially pure aluminium subjected to repeated cold rolling up to an ultra-high accumulated strain ($\epsilon_{eq} = 6.4$) was examined. The deformation path reported in (Mishin et al., 2010, 2013; Delannay and Mishin, 2013) was reproduced: the sheet underwent 54 rolling passes, reducing its thickness from 100 mm to 0.4 mm. The imposed rolling schedule is summarized in Table 4.4, while the roll radius was fixed at 170 mm. ALAMEL was also used for the texture predictions.

4.4 Validation: rolling single material sheet

As outlined in the introduction of this chapter, cold rolling induces pronounced through-thickness strain gradient, which in turn give rise to significant texture heterogeneities. These effects arise from the complex interplay between

Pass	th. red	Pass	th. red	Pass	th. red	Pass	th. red	Pass	th. red	Pass	th. red	Pass	th. red	Pass	th. red
1	0.09	7	0.14	13	0.3	19	0.14	25	0.07	31	0.07	37	0.05	43	0.05
2	0.07	8	0.15	14	0.2	20	0.09	26	0.08	32	0.08	38	0.06	44	0.05
3	0.09	9	0.18	15	0.23	21	0.09	27	0.03	33	0.08	39	0.06	45	0.05
4	0.11	10	0.19	16	0.18	22	0.08	28	0.06	34	0.09	40	0.07	46	0.04
5	0.12	11	0.23	17	0.12	23	0.08	29	0.06	35	0.05	41	0.04	47	0.04
6	0.12	12	0.3	18	0.14	24	0.07	30	0.07	36	0.05	42	0.04	48	0.04

Table 4.4: Rolling schedule showing the prescribed thickness reduction for each pass.

frictional conditions and the roll-gap geometry, characterized primarily by the applied rolling draught. To evaluate the ability of the proposed numerical framework to reproduce this coupled behaviour, its predictions are compared with results reported in the literature. Two configurations are examined: (i) single-rolling pass of a homogeneous sheet under various reductions and friction conditions, and (ii) multi-pass rolling with non-constant rolling draughts.

4.4.1 Single cold-rolling pass of commercially pure aluminium

The influence of the roll-gap geometry on the development of through-thickness strain and texture gradients was first examined.

Modifying the roll-gap geometry altered the manner in which the sheet interacts with the rolls. Figure 4.7 presents the evolution of the normalized contact pressure along the roll-sheet interface for the different roll-gap geometries. For the intermediate and large draughts, the maximum pressure occurred at approximately the same normalized position ($x/l_c \approx 0.64$). In contrast, for the small-draught configuration, the peak pressure shifted toward the entry region ($x/l_c \approx 0.06$). The magnitude of the peak pressure increased with increasing draught, although the cases $l_c/th = 0.5$ and 2 exhibited maxima of comparable magnitude.

The location of the neutral point was identified from the sign change of the contact shear stress shown in Figure 4.8. Upstream of this point, the roll surface velocity exceeded the sheet velocity, giving rise to positive shear stress and, downstream, the relative sliding reversed and the shear stress changed sign. For the intermediate and large draughts, the contact shear stress displayed a sinusoidal-type profile, consistent with earlier numerical predictions for similar rolling conditions (Schoenfeld and Asaro, 1996). In these cases, the neutral point was located between $x/l_c = 0.65$ and 0.77 and the portion of the contact length subjected to negative shear traction increased with increasing draught. The amplitude of the shear stress scaled with the contact pressure. In contrast, for the small-draught configuration, the contact shear remained positive throughout the roll gap, confirming that the neutral point was not reached, in agreement with the behaviour reported for such rolling configuration in (Schoenfeld and Asaro, 1996).

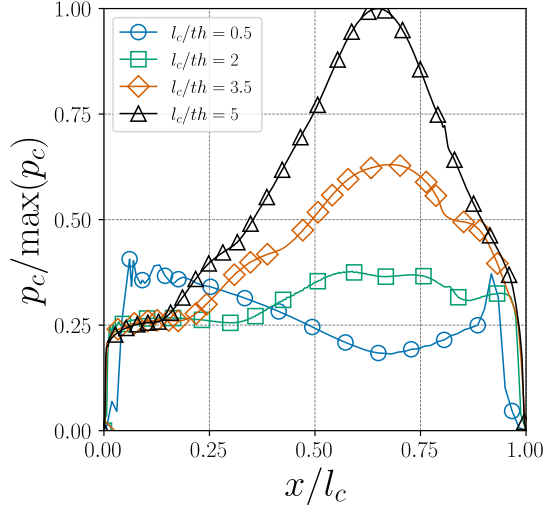


Figure 4.7: Normalized contact pressure p_c along the roll–sheet interface for different roll-gap geometries. The horizontal axis is normalized by the contact length l_c and all curves are normalized by the maximum pressure across the tested configurations. The friction coefficient was identical in all simulations ($\mu = 0.3$).

The final through-thickness shear strain distributions (ε_{13}) for all roll-gap geometries are shown in Figure 4.9. For $l_c/th = 3.5$ and 5, the shear strain remained positive across the thickness and decreased monotonically from the surface toward the centre. These trends are consistent with experimental measurements and numerical predictions under comparable rolling conditions (Choi et al., 1997; Li et al., 2010; Yang et al., 2010). For $l_c/th = 2$, the shear strain decreased from the surface but increased again near $s = 0.5$, in agreement with the trends reported by (Yang et al., 2010). In these three configurations, reducing the draught decreased the magnitude of the shear strain. For the small-draught case, positive shear was confined to the near-surface region, whereas negative shear developed near $s = 0.75$, again consistent with previous predictions (Schoenfeld and Asaro, 1996; Yang et al., 2010). The mid-plane ($s = 0$) remained essentially shear-free in all simulations.

To clarify the origin of these heterogeneous strain fields, the evolution of ε_{13} through the roll gap was analysed for each roll-gap geometry (Figures 4.11–4.14). The shear strain arises from the combined change of F_{31} and F_{13} . As seen in Figures 4.10 and 4.15, the evolution of F_{31} is primarily dictated by roll-gap geometry, whereas F_{13} is controlled mainly by the frictional conditions

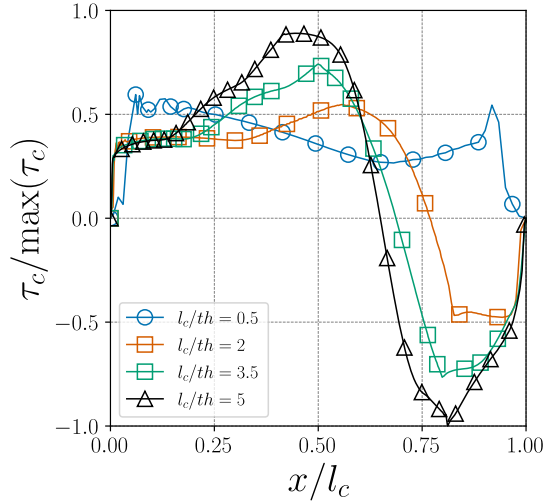


Figure 4.8: Normalized contact shear τ_c along the roll-sheet interface for different roll-gap geometries. The horizontal axis is normalized by the contact length l_c and all curves are normalized by the maximum shear across the tested configurations. The friction coefficient was identical in all simulations ($\mu = 0.3$).

with the rolling mill and the location of the neutral point.

For roll-gap configurations with $l_c/th > 0.5$, friction dominated the shear-strain development. Upon entering the roll gap, the shear strain initially decreased due to increasingly negative values of F_{31} (Figure 4.10). With further penetration, frictional sliding generated large positive contact shear stresses prior to the neutral point (Figure 4.8), while F_{31} progressively approached zero as the material point approached the exit. The combined effect produced a net positive shear strain through the thickness. Increasing the draught amplified the shear strain because both the contact length and the magnitude of the contact shear stress increased. As shown in Figure 4.13, the surface layer ($s = 1$) experienced a sharp reduction in shear strain after passing the neutral point, due to the negative shear stress in this region. This effect was particularly pronounced for $l_c/th = 5$ as surface layer exhibited weaker colouring compared to subsurface layers in Figure 4.9. Similar trends have been reported for large draught configurations in (Schoenfeld and Asaro, 1996).

For the small-draught configuration ($l_c/th = 0.5$), the roll-gap geometry became the dominant factor. Significant shear deformation was required for the material to conform to the entry geometry, producing the highest shear levels reached among all configurations (Figure 4.15). However, because the contact length and frictional shear stresses were both small, shear did not

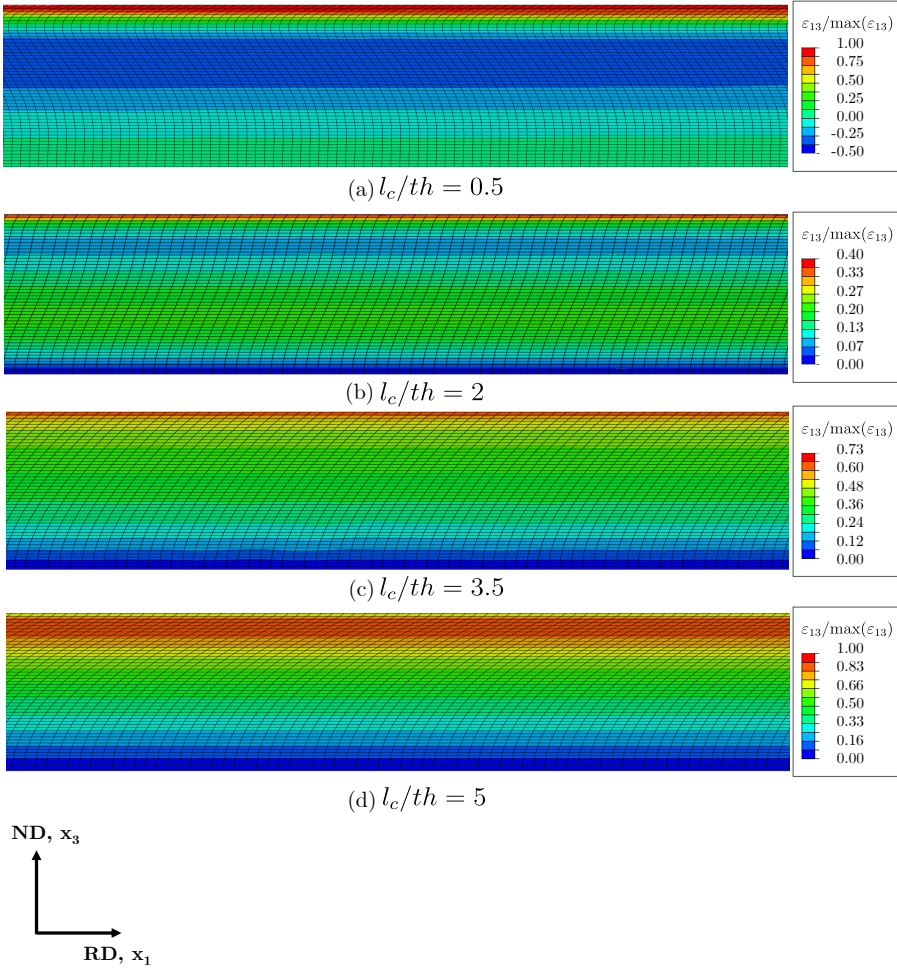


Figure 4.9: Final through-thickness distribution of shear strain (ϵ_{13}) for the different roll-gap geometries. Strains are normalized by $\max(\epsilon_{13})$ observed across all configurations. All simulations were performed with a friction coefficient of $\mu = 0.3$.

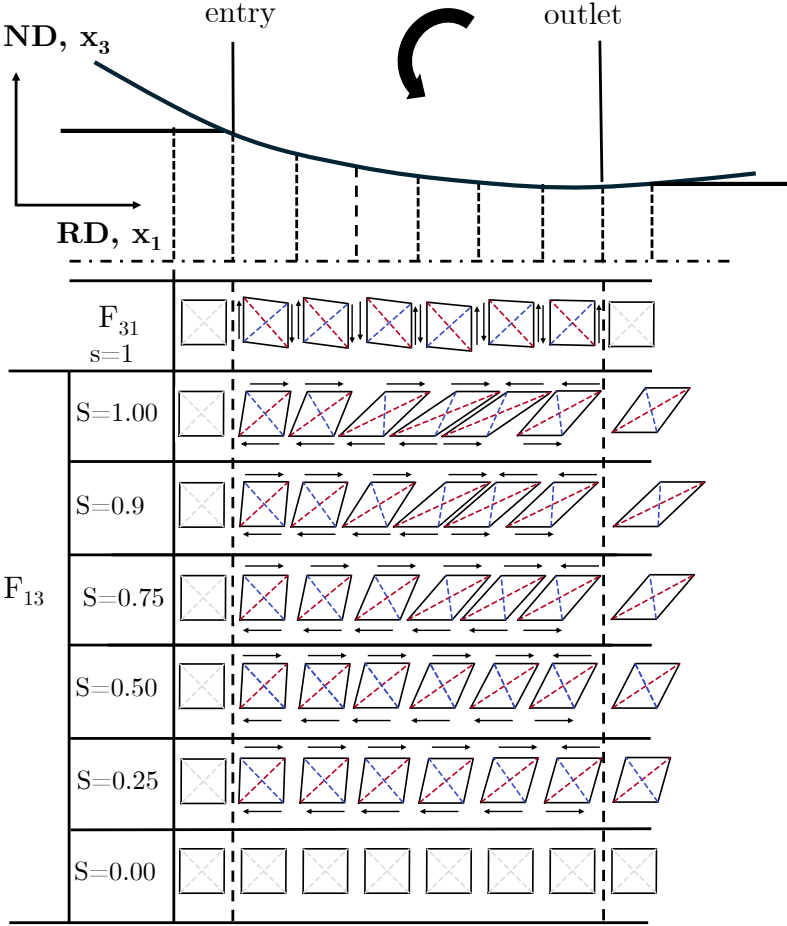


Figure 4.10: Evolution of the deformation gradient components F_{13} and F_{31} for an infinitesimal surface element passing through the roll gap in the large draught configuration $\frac{l_c}{t_h} = 5$. Diagonal colored in blue indicates compression while red indicates tension. This figure is adapted from (Engler et al., 2000).

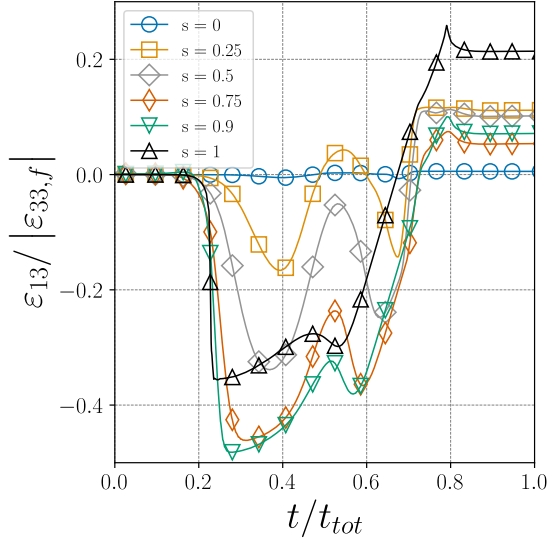


Figure 4.11: Normalized shear strain $\varepsilon_{13}/\varepsilon_{33,f}$ as a function of normalized time t/t_{tot} for $\frac{l_c}{t_h} = 2$ and friction coefficient $\mu = 0.3$. Here, $\varepsilon_{33,f} = -0.69$ denotes the final plastic strain in the normal direction and t_{tot} is the total simulation time.

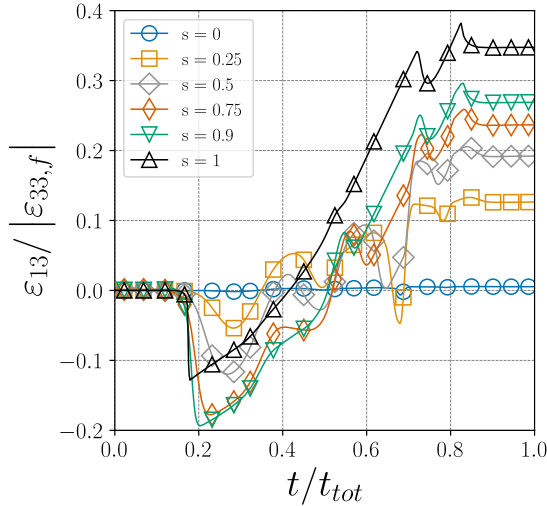


Figure 4.12: Normalized shear strain $\varepsilon_{13}/\varepsilon_{33,f}$ versus normalized time t/t_{tot} for $\frac{l_c}{t_h} = 3.5$ and friction coefficient $\mu = 0.3$. Here, $\varepsilon_{33,f} = -0.69$ denotes the final plastic strain in the normal direction and t_{tot} is the total simulation time.

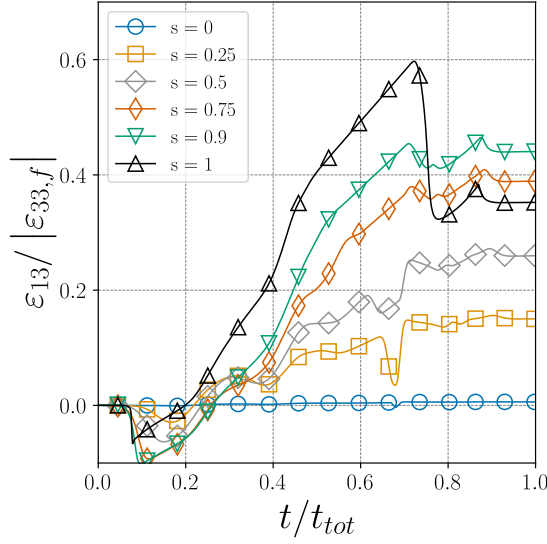


Figure 4.13: Normalized shear strain $\varepsilon_{13}/\varepsilon_{33,f}$ versus normalized time t/t_{tot} for $l_c/th = 5$ and friction coefficient $\mu = 0.3$. Here, $\varepsilon_{33,f} = -0.69$ denotes the final plastic strain in the normal direction and t_{tot} is the total simulation time.

penetrate deeply. Indeed, only the surface and subsurface layers accumulated positive shear strain, while layers below $s \leq 0.75$ developed negative shear. This result aligns with the numerical predictions of (Schoenfeld and Asaro, 1996) for small-draught configuration.

Across all rolling configurations, the centre of the sheet ($s = 0$) remained nearly shear-free throughout, supporting the common assumption of near plane-strain compression in this region.

The heterogeneous shear deformation produced pronounced through-thickness texture gradients, as shown in Figure 4.17. In all configurations, the textures evolved between the classical copper-type components (whose ideal components are shown in Figure 4.16.a) and the shear-type components (Figure 4.16.b). The transition between these sets of components occurred primarily through rotations about the transverse direction (TD), consistent with experimental observations (Kim and Lee, 2001; Sakai et al., 2001).

For geometries with $l_c/th > 0.5$, copper-type texture dominated near the sheet centre, gradually rotating toward shear-type components toward the surface. The degree of TD-axis rotation was directly correlated with the local magnitude of the shear strain ε_{13} . For example, at $s = 0.5$, the rotation increased systematically with increasing the rolling-draught, reflecting the higher shear levels predicted for these positions. The depth of shear penetration was also evident: the texture at $s = 0.75$ for $l_c/th = 2$ closely resembled

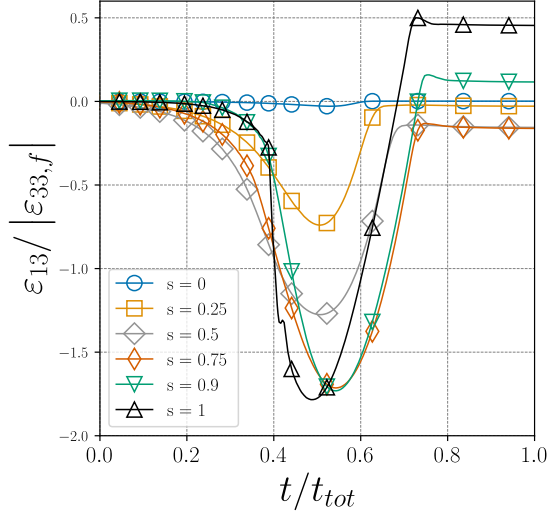


Figure 4.14: Normalized shear strain $\varepsilon_{13}/\varepsilon_{33,f}$ versus normalized time t/t_{tot} for $\frac{l_c}{th} = 0.5$ and friction coefficient $\mu = 0.3$. Here, $\varepsilon_{33,f} = -0.69$ denotes the final plastic strain in the normal direction and t_{tot} is the total simulation time.

that at $s = 0.5$ for $l_c/th = 5$, consistent with the deeper shear penetration at larger draughts, as shown in Figures 4.11 and 4.13. Shear textures near surfaces were already observed experimentally for similar rolling conditions supporting these results (Truszkowski et al., 1980). It is interesting to note that, contrary to some literature claims (Mishin et al., 2000), intermediate draughts as $l_c/th = 3.5$ produced strain heterogeneity comparable to that obtained in large draught case.

For $l_c/th \leq 0.5$, nearly pure copper-type textures were predicted at the sub-surface position ($s = 0.9$), while layers in the range $0.25 \leq s \leq 0.75$ exhibited an inverse TD-axis rotation. This behaviour is consistent with the presence of negative shear strains in these regions and with the transition from positive to negative shear occurring near $s \approx 0.9$. These predictions aligned with previous numerical and experimental results for this rolling draught (Truszkowski et al., 1980; Schoenfeld and Asaro, 1996).

The second parameter identified as governing strain heterogeneity was the friction coefficient. Its influence was assessed by varying the coefficient of friction while keeping the roll-gap length constant ($l_c = 5$). The results indicate that, although friction did not modify the qualitative evolution of the strain during the rolling pass, it strongly affected the magnitude of the shear strain across the sheet thickness. As shown in Figure 4.18, increasing the friction coefficient enhanced the shear strain at all thickness positions,

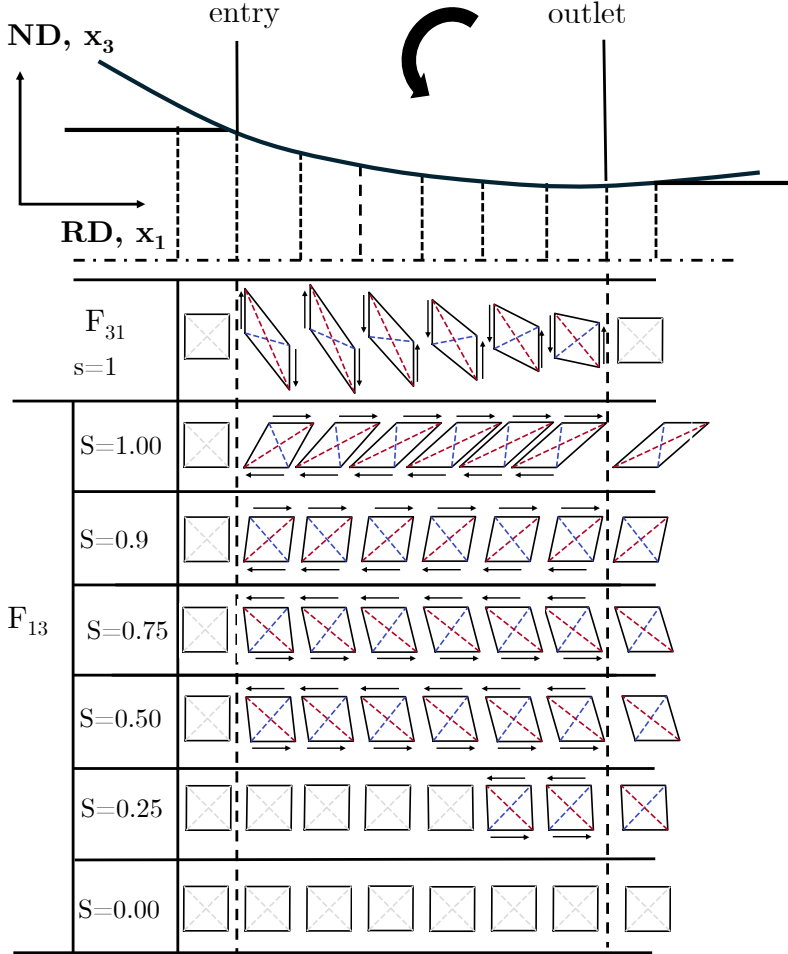


Figure 4.15: Evolution of the deformation gradient components F_{13} and F_{31} for an infinitesimal surface element passing through the roll gap in the small draught configuration $\frac{l_c}{t_h} = 0.5$. Diagonal colored in blue indicates compression while red indicates tension. This figure is adapted from (Engler et al., 2000).

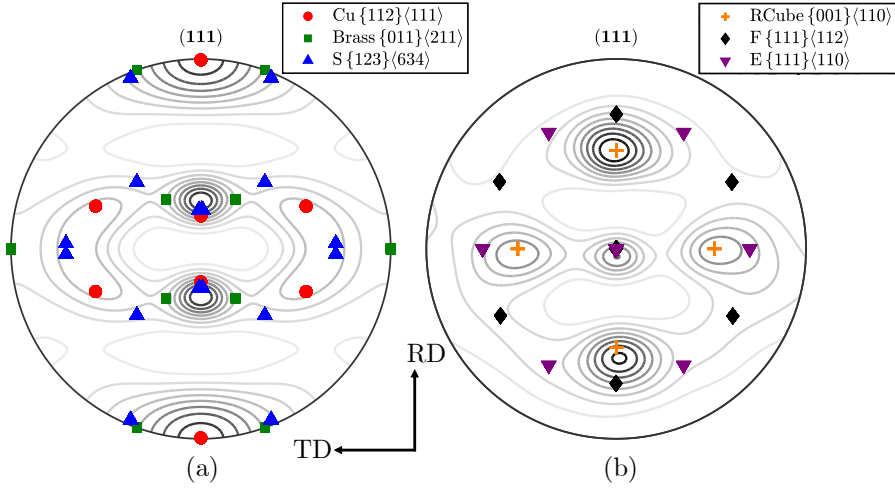


Figure 4.16: Ideal orientations of the principal texture components observed during cold rolling: (a) copper-type texture (Copper, Brass, S) and (b) shear-type texture (Rotated Cube, E, F), represented in the $\{111\}$ pole figure in the RD-TD plane.

whereas reducing the coefficient decreased the overall shear level.

These trends reflected directly in the texture evolution. Figure 4.19 shows that higher friction coefficients promoted larger rotations around the transverse direction (TD) axis throughout the thickness. Indeed, higher friction increased the magnitude and penetration depth of shear, thereby inducing greater lattice rotation at a given thickness position. For instance, the texture measured at $s = 0.5$ exhibited progressively greater TD-axis rotation as the friction coefficient increased. These observations are consistent with previous experimental and numerical studies on frictional effects in cold rolling (Choi et al., 1997; Huh et al., 1999; Kang et al., 2007; Chen et al., 2011; Cantergiani et al., 2024).

Overall, these results confirmed that the proposed numerical framework accurately captured the complex interplay between frictional effects and roll-gap geometry during a single cold-rolling pass. The agreement with experimental observations and with predictions from more advanced numerical models confirms the robustness of the approach and the correct implementation.

4.4.2 Multiple cold-rolling pass of commercially pure aluminium

As shown in Figure 4.20, the rolling schedule maintained the roll-gap geometry predominantly within the intermediate-draught regime, in agreement with

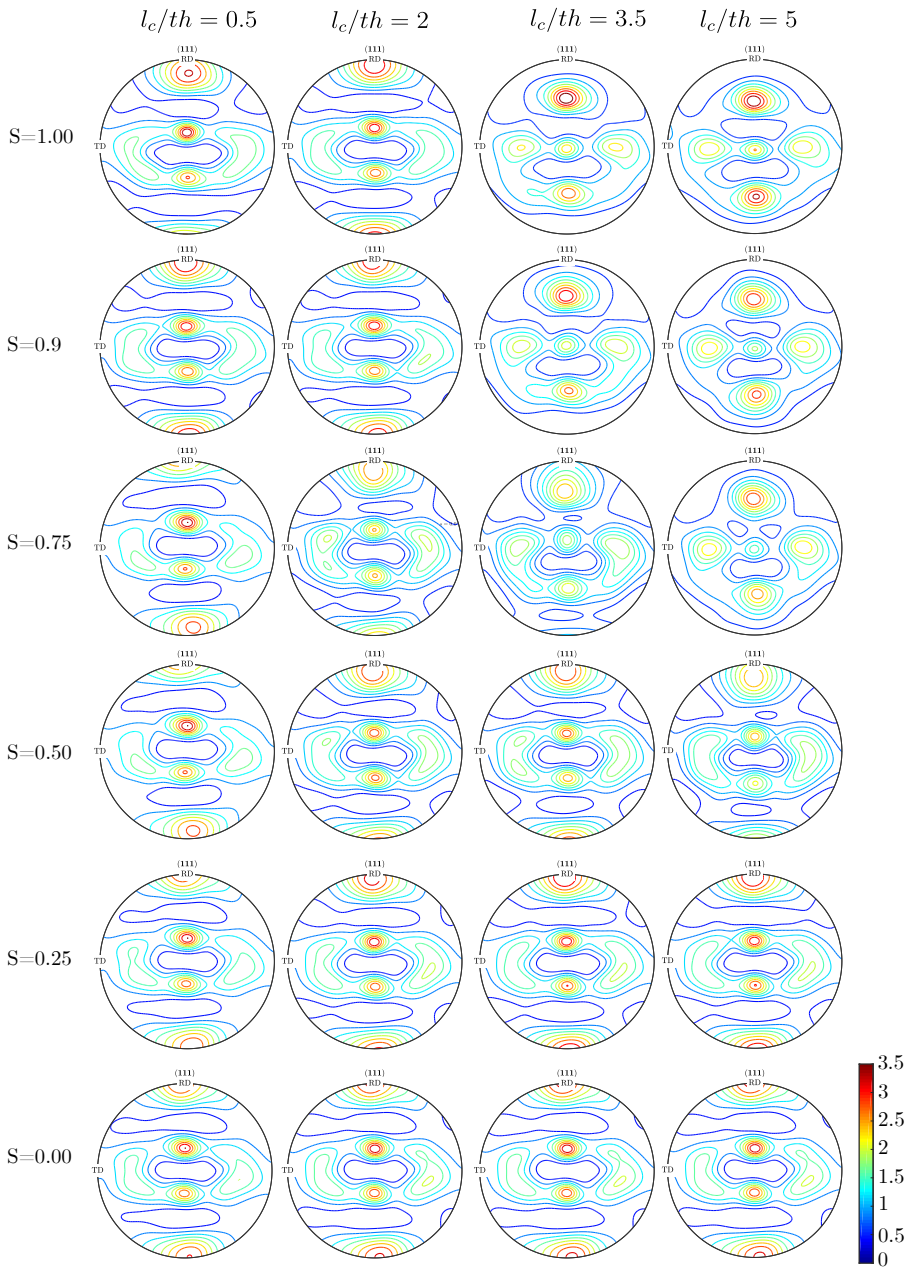


Figure 4.17: Comparison of $\{111\}$ pole figures in the RD-TD plane for different roll-gap geometries and thickness positions. All simulations were performed with a friction coefficient of $\mu = 0.3$.

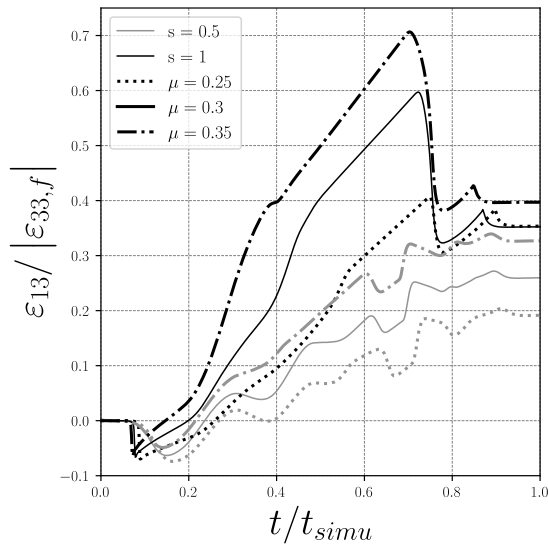


Figure 4.18: Normalized shear strain $\varepsilon_{13}/\varepsilon_{33,f}$ as a function of normalized time t/t_{tot} for the roll gap configuration $\frac{l_c}{th} = 5$, for several values of the friction coefficient.

		Cu	S	Brass
Centre	Experimental	28%	53%	15%
	Simulation	24%	39%	0%
Subsurface	Experimental	50%	38%	4%
	Simulation	57%	15%	1%

Table 4.5: Experimentally measured (Mishin et al., 2013) and predicted volume fractions of the main texture components at the central and subsurface regions.

the experimental conditions (Mishin et al., 2010, 2013). However, throughout the 54 passes, the process covered a broad range of roll-gap configurations, initially corresponding to a small-draught configuration and progressively approaching the large-draught configuration.

Only the final textures at the subsurface and central regions were probed experimentally. Figure 4.21 compares the predicted and measured $\{111\}$ pole figures at both locations, showing a good qualitative agreement. The corresponding volume fractions of the main texture components are listed in Table 4.5.

In both regions, the dominant orientations were the Copper $\{112\}\langle 111\rangle$, S $\{123\}\langle 634\rangle$, and Brass $\{110\}\langle 112\rangle$ components. At the subsurface, the S component intensity was slightly underpredicted by the model, while at the

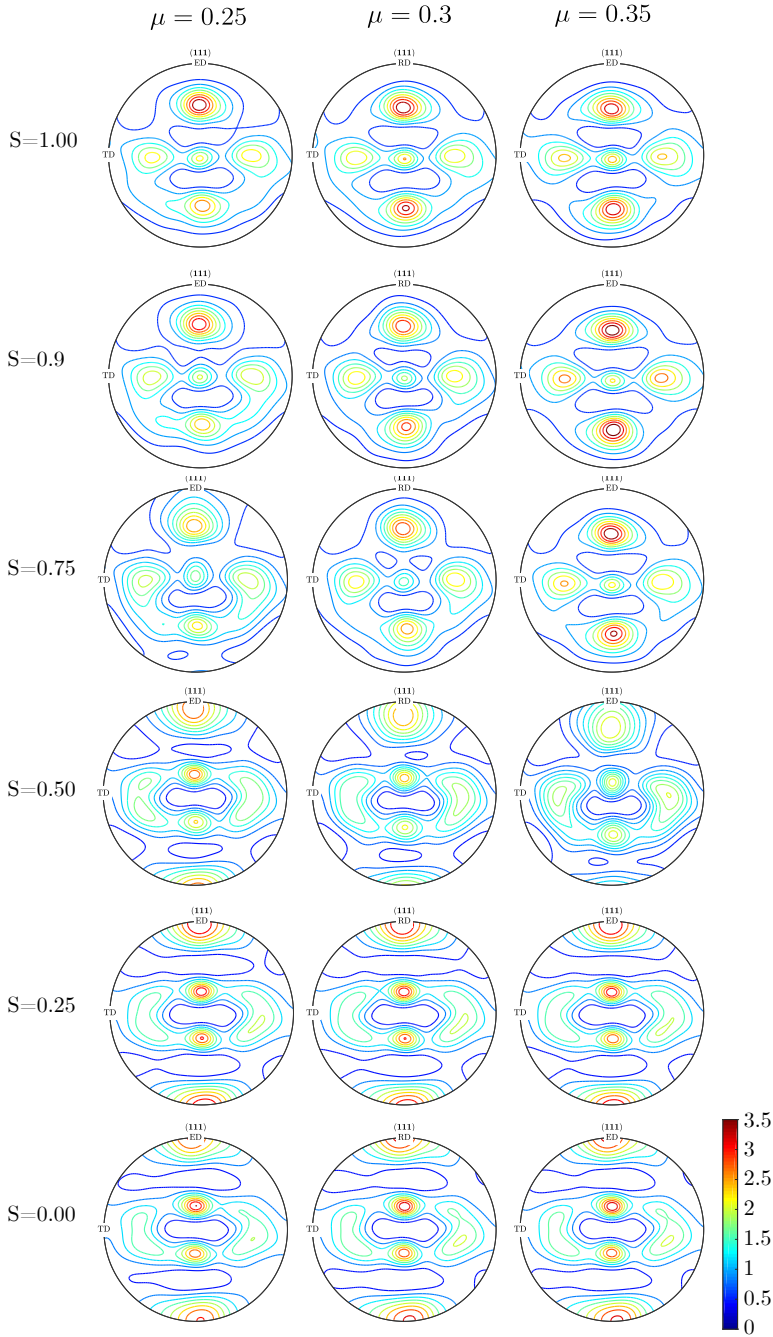


Figure 4.19: Comparison of $\{111\}$ pole figures in the RD-TD plane for different friction coefficients and through-thickness positions. All simulations were performed using the same roll-gap geometry $l_c/th = 5$.

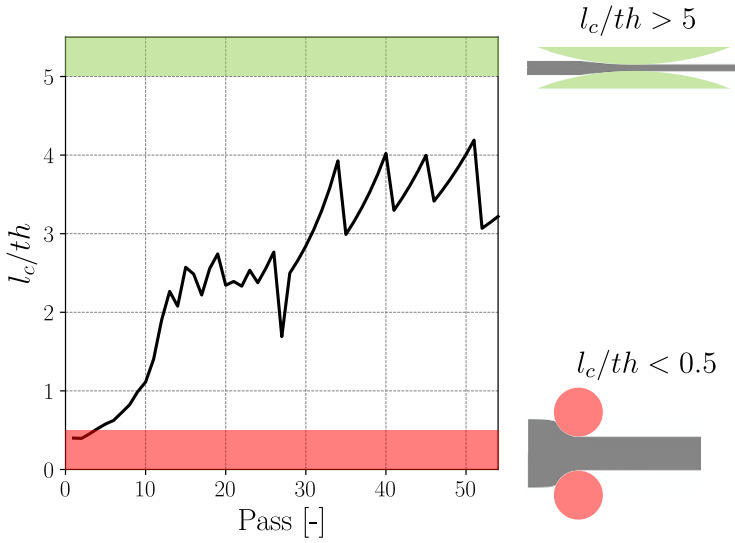


Figure 4.20: Evolution of the rolling draught over the 54 rolling passes. The red region denotes the small-draught regime, while the green region corresponds to the large-draught regime.

sheet center both the S and Brass components were underestimated. These deviations can be attributed to the initial through-thickness texture gradient present in the experimental material but not considered in the simulations. In the experiments, the central region already exhibited a pronounced rolling texture, with initial volume fractions of Brass and S components of 13% and 23%, respectively, which is far from negligible, while a shear-type texture was initially present near the subsurface (Mishin et al., 2010, 2013). In contrast, the simulations assumed a random initial orientation distribution throughout the thickness.

Despite the absence of this initial texture gradient, the simulated textures reproduced the main experimentally observed crystallographic components and captured the relative intensities with reasonable accuracy. These results confirm the robustness of the proposed numerical framework and its suitability for simulating accumulative cold-rolling processes involving very large equivalent strains.

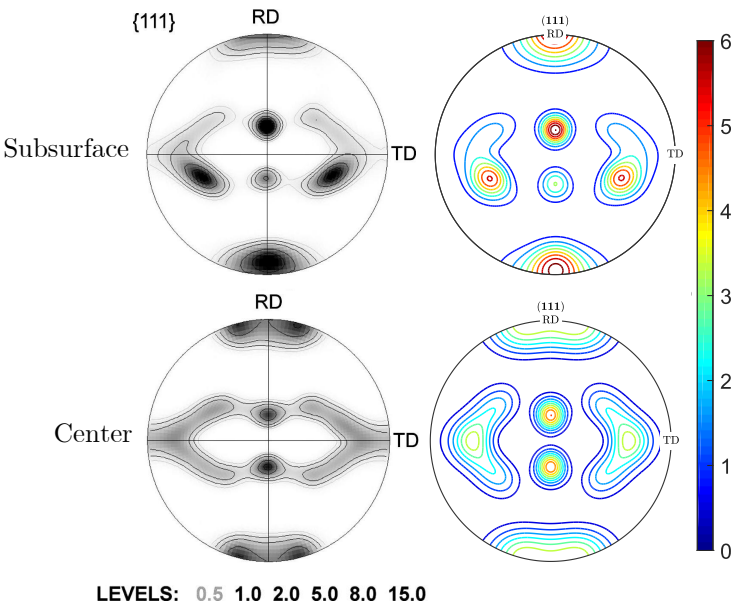


Figure 4.21: RD-TD $\{111\}$ pole figures representing the textures at subsurface and central regions measured experimentally (Mishin et al., 2013) and predicted by the numerical framework after 54 rolling passes.

F_{12}/F_{11}	S=0	S=0.37	S=0.75
Fe	0	0.75	1
Fe-Al	0	7	0.19

Table 4.6: Ratio between the resulting shear component F_{12} and the elongation component F_{11} after cumulating the two passes, evaluated at different normalised through-thickness positions. These three positions correspond to the locations of the three layers in the final configuration. “Fe” refers to the case where iron is considered as the unique constituent, while “Fe–Al” denotes the configuration accounting for the presence of an aluminium layer.

4.5 Results

4.5.1 5-layers Fe-Al multi-laminate

Simulations revealed that the introduction of aluminium layers strongly modified the through-thickness distribution of shear strain. As shown in Figure 4.22 a. and b., shear deformation was strongly localized within the aluminium layers during both passes, instead of spreading across the whole sheet thickness as commonly observed in large roll-gap configurations (Figure 4.22(c)). For both passes, the peak shear component of the deformation gradient within the aluminium layers reached values up to six times higher than those predicted for a homogeneous material subjected to the same rolling draught.

The harder Fe layers were far less affected by shear. After the first pass, the central Fe layer exhibited shear levels similar to those predicted at this position in the single-material reference configuration. During the second pass, only a moderate amount of shear developed within the outer Fe layers, while the central Fe layer experienced no additional shear.

The final deformation-gradient ratio F_{12}/F_{11} , reported in Table 4.6, emphasizes the strong influence of the presence of the softer aluminium layers, which significantly modified the local shear distribution. This pronounced localization results from the large contact length (about 10 times the thickness of the sample) between the rolls and the plate which induces substantial contact shear stresses, and the significantly lower yield stress of aluminium compared with iron.

Using the layer-specific deformation paths obtained from the macroscopic simulations for both passes, crystal plasticity (CP) modelling was employed to predict texture evolution. The resulting $\{111\}$ poles figures are shown in Figure 4.23, in direct comparison with the experimental textures presented in Figure 4.3. The surface Fe layer was disregarded as the experimental texture was very weak, a consequence of the limited thickness reduction experienced during the final pass. The predicted central Fe layer exhibits a typical rolling-

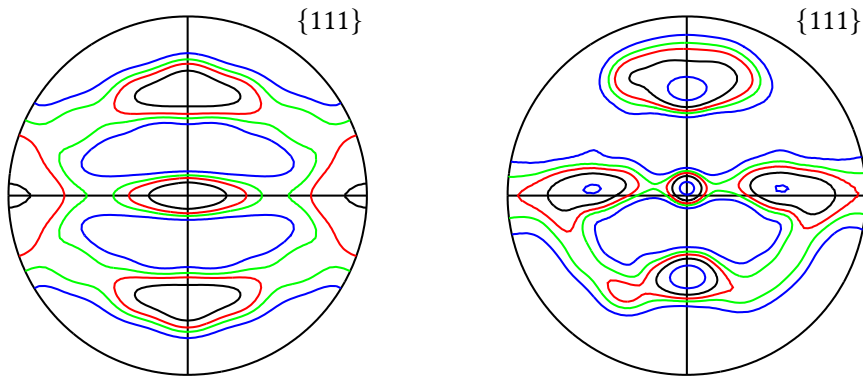


Figure 4.23: $\{111\}$ pole figures in the RD-TD plan predicted in the central Fe layer (a) and in the AA1050 layer (b). The contour levels are 0.5/1/1.5/2/5.

type texture with orthorhombic symmetry, whereas the aluminium layer show features representative of shear texture. The orientation distribution function (ODF) allows a more accurate comparison of the predicted textures to the experimental ones. For rolled cubic metals, the most relevant information lies in the $\varphi_2 = 45^\circ$ section of the ODF, shown in Figure 4.24. For the central iron layer, both experimental and predicted ODF are characterised by a strong γ -fibre and a partial α -fibre. In the aluminium layer, distinct components such as $(111)[\bar{1}10]$, $(111)[\bar{1}\bar{1}0]$, $(111)[\bar{1}21]$, and the $\{011\}\langle 110 \rangle$ family (corresponding to the rotated cube, S, and F orientations typically associated with shear deformation in FCC metals) appear in both the measurements and the predictions, as shown in Figure 4.24. The close agreement between predicted and experimentally measured textures in both layers confirms the validity of the predictions in both layers.

4.5.2 9-layers Fe-Al multi-laminate

Macroscopic simulations of Passes 1 and 2 are shown in Figures 4.22.a and 4.25. As in the five-layer laminate, significant shear deformation parallel to the rolling plane was predicted in the aluminium layers during both passes. Due to the symmetry, the two outer aluminium layers exhibit identical shear levels after the first pass. However, their final strain states differ in the nine-layer multi-laminate: the outermost aluminium layer undergoes the most intense shear during the second pass, resulting in a final shear component F_{12} nearly four times larger than that of the innermost layer. Concerning the iron layers, although the shear magnitudes are significantly lower, the largest final shear strain is located at quarter-thickness rather than in the external Fe layer,

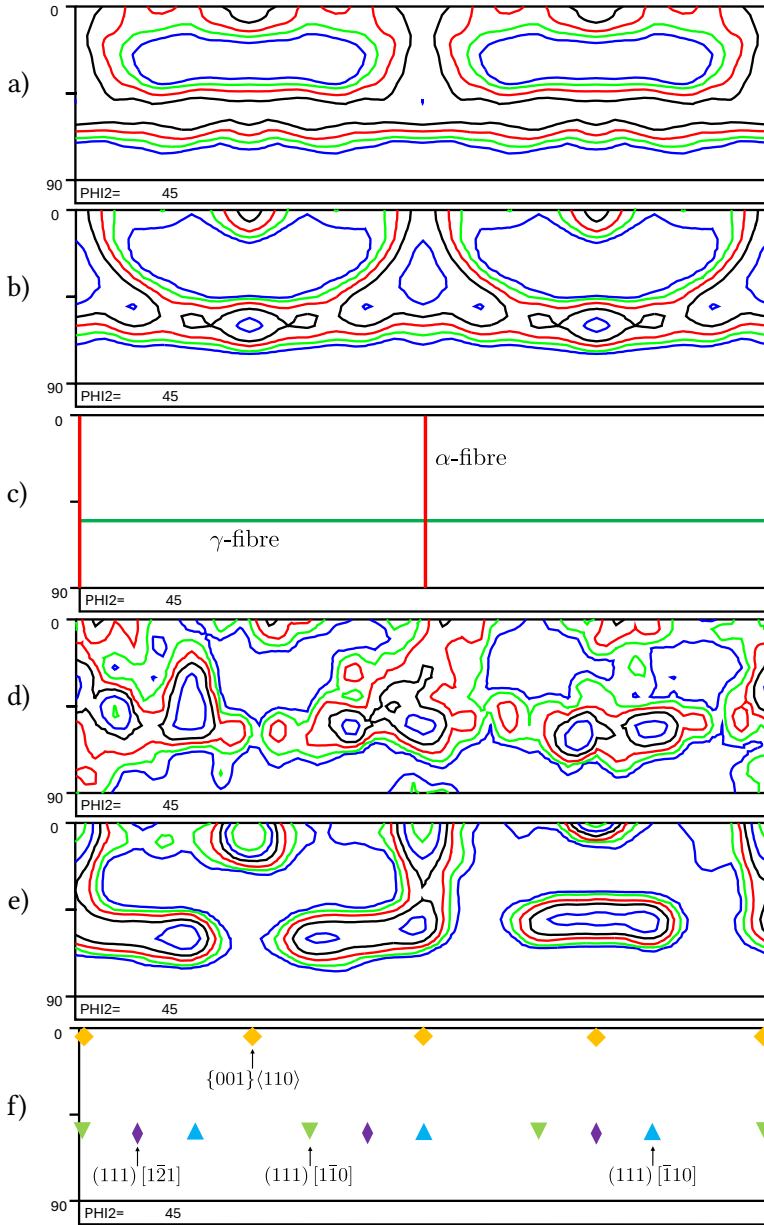


Figure 4.24: $\phi_2 = 45^\circ$ section of the ODF allowing a quantitative assessment of the experimental (a) and predicted (b) textures in the central Fe layer. The positions of the ideal crystallographic fibres associated with rolling textures in BCC metals are shown in(c). The experimental (d) texture in AA1050 is compared to predictions which use the strain predicted by FE (e). The positions of the ideal texture components characteristic of shear textures in FCC metals are indicated in (f). The contour levels are 0.5/1/2/4/8.

F_{12}/F_{11}	$S=0$	$S=0.25$	$S=0.4$	$S=0.6$	$S=0.83$
Fe-Al	0	1.77	0.25	9	0.2

Table 4.7: Ratio between the resulting shear component F_{12} and the elongation component F_{11} after cumulating the two passes, evaluated at different normalised through-thickness positions. These positions correspond to the locations of the five layers in the final configuration. The positions $S = 0.25$ and $S = 0.60$ correspond to aluminium layers, while the remaining positions correspond to iron layers.

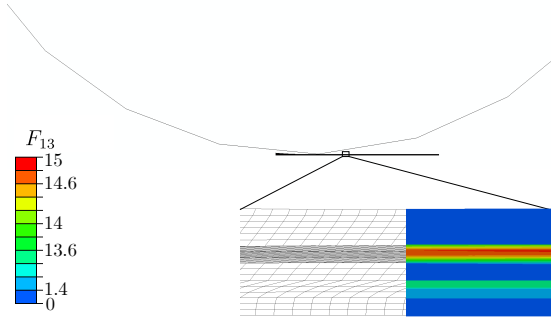


Figure 4.25: The macroscopic through thickness strain distribution was predicted during the 2nd rolling pass. The corresponding deformed mesh is displayed alongside the RD-ND shear strain map.

which would be expected for such rolling draught. A shear-strain gradient is therefore expected between the central Fe layer and the other Fe layers. All these trends are clearly reflected in Table 4.7.

Macroscopic FE model did not predict the emergence of deformation instabilities observed experimentally, such as the formation of inclined shear bands. These shear bands are expected to locally modify the strain distribution and to influence texture development. Therefore, we considered that the deformation inside each layers was a combination of three different deformation modes: ND-RD plane strain compression, shear parallel to the rolling plane and shear banding tilted at 45° from the rolling direction. In all cases, boundary conditions were prescribed to achieve a consistent von Mises equivalent strain of 0.5.

As shown in Figure 4.26, shear parallel to the rolling plane induces anti-clockwise rotation ($\sim 15^\circ$) of the pole figures that were predicted under orthotropic plane strain compression. Indeed, such shear is equivalent to compression along a direction that is inclined relative to RD. It is noteworthy that the (anticlockwise) rotation of the compression axis is opposite to the

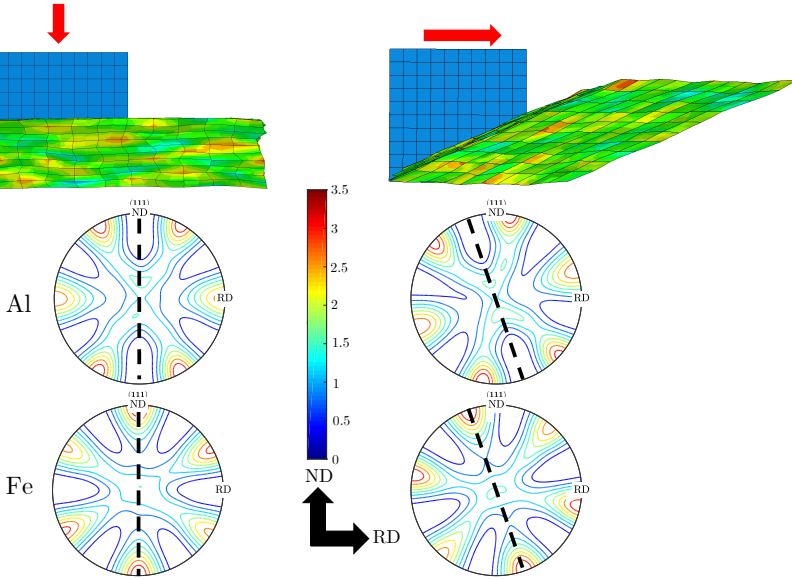


Figure 4.26: Compression and shear deformation modes. Textures predicted to develop inside Fe or Al are presented as $\{111\}$ pole figures.

(clockwise) spin expected from shearing.

As shown in Figure 4.27, the effect of shear bands inclined at $\pm 45^\circ$ to the rolling direction is different. Such shear banding is equivalent to the superposition of orthotropic plane strain compression with rigid body rotation. The comparison of Figure 4.26.a. and Figures 4.27 shows that the pole figure rotation now conforms to the spin inside the shear band.

The experimental pole figures shown in Figure 4.4 are representative of the mean texture in each layer so that the local effects of shear bands are suppressed. Based on the results presented in this section, Figure 4.28 indicates, in a qualitative manner, the type of shear expected, respectively, in the upper and lower layers of the multi-laminate.

4.6 Discussion

Orientation mapping (based on EBSD measurements) is a powerful experimental technique which allows probing both the texture and the microstructure in the different layers of the multilaminate (Figures 4.3 and 4.4). However, the technique does not provide direct measurements of the microscopic strain field (unless it is combined with DIC as in Lin et al. (2018)). The present study demonstrates that numerical modelling can effectively support and enrich the

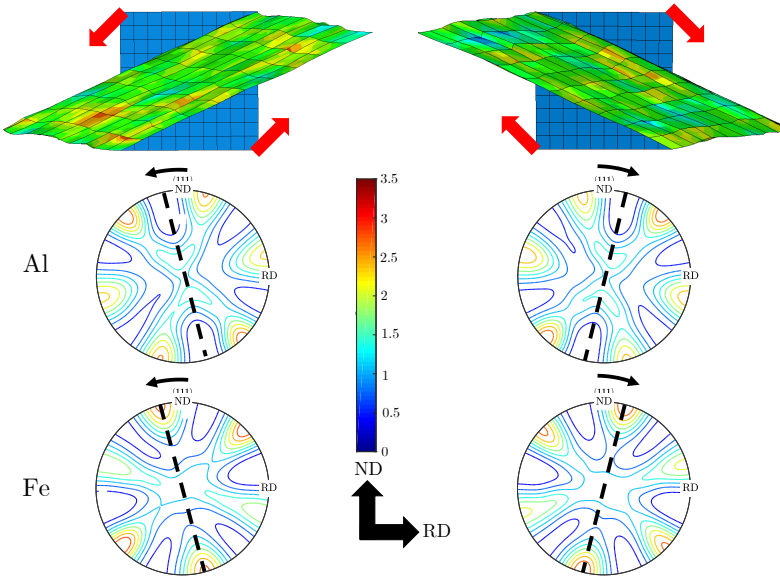


Figure 4.27: Positive shear band and negative shear band modes. Textures developed inside Fe or Al microstructures are presented as $\{111\}$ pole figures.

interpretation of orientation maps. A multiscale numerical framework was developed by coupling two numerical models operating at different length scales, enabling a direct link between the local strain field and the evolution of crystallographic texture during one or multiple rolling passes. The framework was validated through comparison with results available in the literature. Compared to a fully coupled approach (CPFEM directly used to simulate rolling), the suggested uncoupled macro- and micro-modelling is computationally efficient, provides greater flexibility, and facilitates the interpretation of more extreme cases (large number of rolling passes or emergence of layer instabilities).

In the 5-layer multi-laminate, it is through the combined use of the experimental textures and the numerical models that we are able to confirm that the AA1050 layer underwent intense shear, causing continuous recrystallization as well as the development of an unconventionally strong shear texture after cold rolling. Such texture accompanied with grain refinement are generally observed in asymmetric rolling where important plastic shear strain is induced (Cui and Otori, 2000; Lee, 2004; Lee and Lee, 2008). In the 9-layer multi-laminate, EBSD measurements in aluminium revealed also a refined microstructure but having a different texture: a weak $\{\bar{1}10\}$ $\langle 110 \rangle$ component. Such texture was already reported inside pure aluminium and were formed

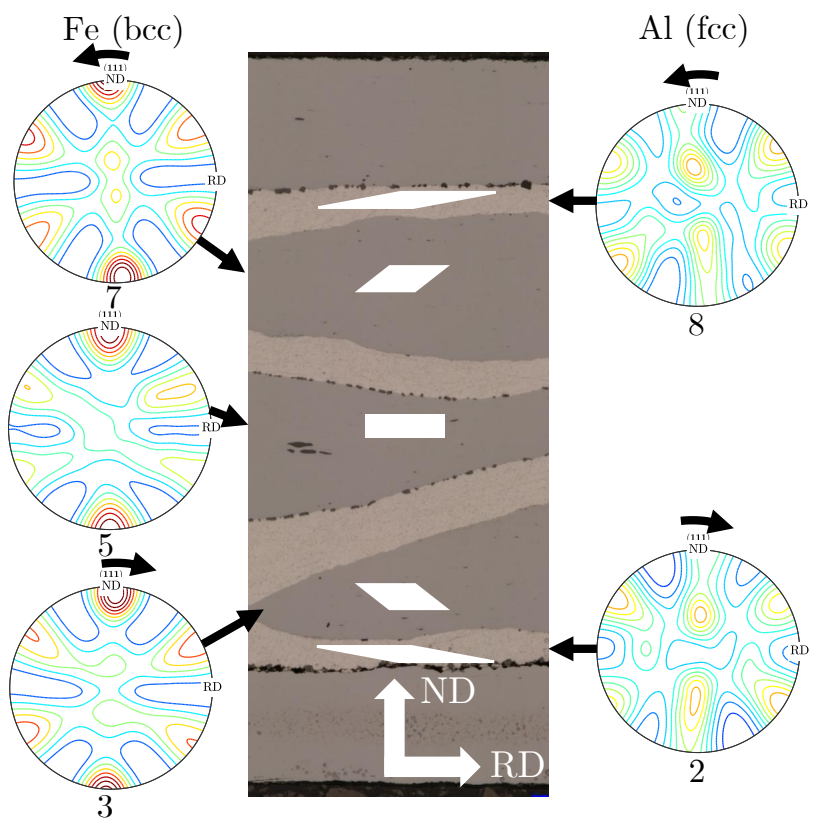


Figure 4.28: When considering shear parallel to the rolling plane, crystal plasticity predictions provide fair reproduction of the average texture inside each layer. The black arrows highlight the slight rotations relative to the orthorhombic texture expected under plane strain compression.

from the C {001} <110> component (shear texture component illustrated in Figure 4.16.b) through continuous recrystallization due to intense shear deformation (Li et al., 2022). This too conforms to the prediction of the macroscopic FE model. However, crystal plasticity simulations failed to capture the specific texture transition observed in the 9-layer case. This discrepancy highlights the persisting challenges in accurately predicting texture evolution in FCC metals subjected to severe plastic deformation.

In both multi-laminates, textures in all the Fe layers are close to conventional rolling textures predicted under plane strain compression. However, for the 9-layer multi-laminate, they are slightly rotated ($\sim 5^\circ$) around the transverse direction, with opposite signs on either side of the mid-thickness. Such rotations are typically associated with the development of shear textures (Sakai et al., 2001; Kim and Lee, 2001). This is consistent with the predictions of the macroscopic FE model: there is moderate shear parallel to the rolling plane in the hard phase. Note that the amplitude of rotation is much smaller than predicted in Figure 4.26 since compression and shear occurred simultaneously in the real plate. The texture observed in the central iron layer was orthorhombic indicating that shear was close to zero.

As previously demonstrated for rolled single-material sheets, texture evolution can provide valuable insight into the macroscopic through-thickness strain distribution in multilaminates produced by accumulative roll bonding. This finding highlights the potential of macroscopic texture analysis when aiming to identify the presence of strain gradients, by exploiting the rich information contained in orientation maps. To further illustrate this potential, a similar analysis was carried out on a roll-bonded multilayer composed of stainless steels 316L and AISI 410. Based solely on texture measurements, the results indicate the presence of a through-thickness shear gradient, with shear magnitude increasing progressively away from the mid-plane. These measurements also suggest that none of the layers accumulated significant shear strain, in contrast to the behaviour observed in the Fe–Al system. Further details are provided in Appendix B.

Nevertheless, additional investigations are needed to assess the robustness of the approach under different rolling conditions. The Fe–Al multilaminates studied here were characterised by initially untextured layers and were subjected exclusively to large rolling draughts during the two roll-bonding passes. Under these conditions, the proposed methodology performs well. However, intermediate or small rolling draughts, as well as mixed draught sequences, are expected to generate different strain gradients, as illustrated in this chapter, and therefore require further validation. Similarly, pronounced initial textures in the constituent sheets would likely complicate interpretation and would require dedicated analysis.

A natural extension of this work is to evaluate the extent to which local texture measurements may be used to determine the local plastic strain field. The ideal scenario would be to reconstruct the strain distribution directly from the spatial variation of texture. In practice, however, interpreting local textures can be challenging. Two representative examples from non-planar layers in the 9-layer multi-laminate studied illustrate this difficulty (see Appendix C). In these examples, the apparent rotation of the pole figure was not caused by shear deformation but by rigid-body rotation associated with layer shrinkage or undulation. Further studies are required to assess the feasibility of this approach across different length scales.

4.7 Conclusion

In this chapter, the use of crystallographic texture to identify and characterize the strain heterogeneity developing within multilayered sheets composed of commercially pure aluminium and iron produced by accumulative roll bonding (ARB) has been investigated. The main conclusions are summarized as follows:

- A multiscale numerical framework was developed to link the through-thickness strain and texture evolution during cold rolling. The model was extended from single-pass to multi-pass rolling simulations. The predictions were successfully validated against data reported in the literature for bulk Al sheets.
- The comparison of experimental textures to the predictions obtained in multi-laminates (macroscopic strain fields and microscopic texture) allowed us to convincingly link the EBSD observation of the different layers to the through-thickness strain heterogeneity predicted by FE modeling.
- The two Fe-Al multilaminates studied had a very different through-thickness strain gradients than those predicted for a homogeneous material rolled with a large rolling-draught. The softer AA1050 layers hosted intense shear parallel to the rolling plane, irrespective of their position within the stack, with shear magnitudes sufficient to promote continuous recrystallization. In contrast, the iron layers were subjected predominantly to orthotropic plane-strain compression near the mid-thickness, while only moderate shear deformation developed toward the outer regions.

Microscopic strain heterogeneity inside individual grains

5

After examining macroscopic strain and texture heterogeneities in extruded and rolled metallic sheets in the previous chapters, the present chapter focuses on the deformation heterogeneity within individual crystals. The mean-field models employed previously provided valid predictions while relying on simplifying assumptions regarding grain-scale micromechanics. It is therefore of interest to assess the extent to which intragranular deformation deviates from these assumptions. This chapter aims to characterize deformation heterogeneities at the microscale and on the role played by crystalline interfaces in the development of these heterogeneous fields. A thorough understanding of these heterogeneities is essential, as they strongly influence macroscopic failure arising from strain localization and crack initiation at the micro-scale. To this end, the chapter also investigates a novel approach aimed at predicting microscale deformation heterogeneities.

The chapter is organized as follows. Introduction section reviews the state-of-the-art in both the experimental observation and the modelling of microscopic strain heterogeneity. Section 5.2 presents an analysis based on CPFEM simulations to deepen the understanding of micro-scale strain fields and to measure the influence of proximity to crystalline interfaces. Building on these findings, Section 5.3 introduces a novel CPFEM-based strategy designed to account for interface-induced heterogeneity. The performance of this approach is then assessed against a more conventional modelling framework. The results are discussed in Section 5.4, followed by concluding remarks.

The work presented in this chapter is the subject of a journal article in preparation for International Journal of Plasticity:

- **Hanon, G.**, Delannay, L., Modeling the influence of crystalline interfaces on the microscopic strain heterogeneity

5.1 Introduction

According to both experiments and numerical models, microscopic strain and stress fields exhibit significant heterogeneity within polycrystals. It is widely acknowledged that such heterogeneity arises due to crystalline interfaces, which act as obstacles to dislocation motion, and the inherent anisotropy of the constituent grains. However, several fundamental questions remain subjects of ongoing debate (McDowell, 2010), such as the relationship between plastic deformation and the distance to crystalline interfaces, the influence of these interfaces on slip system activity, and the nature of the interaction of adjacent grains across crystalline interfaces. This study aims to address these questions and propose a novel, computationally efficient, approach for Crystal Plasticity Finite Element Method (CPFEM) integrating the interactions with neighbouring grains.

Experimental Digital Image Correlation (DIC) techniques have revealed the highly heterogeneous nature of deformation within polycrystals. DIC is currently widely used to track and map the strain distribution on the surface of deformed polycrystals (McMurtrey et al., 2014; Tasan et al., 2014; Di Gioacchino and Quinta da Fonseca, 2015; Zhang et al., 2018; Ren et al., 2021; Shang et al., 2021). Early work on recrystallized aluminium sheet revealed a systematic tendency for strain to localize in the vicinity of grain boundaries (Raabe et al., 2001). Similar observations were later reported for magnesium alloys, where the local plastic strain rate near grain boundaries was measured to be up to 32 times higher than the applied macroscopic value (Orozco-Caballero et al., 2017). In a commercial ZEK100 alloy, it was reported that the amplitudes of equivalent plastic strain and of tensile strain had a larger range of variation when probed near grain boundaries (Sinclair et al., 2014; Martin et al., 2014). They also reported that the largest and the smallest strain amplitudes were always located near grain boundaries. It is important to note that these two last studies focused solely on the distribution of local strain as a function of the distance to the nearest grain boundary, without attempting to extract a general trend of the strain level and the distance to the crystalline interface from the raw data.

Nanoindentation testing allows probing the heterogeneity of the hardness over a surface of interest (Lee and Chen, 2010; Goto et al., 2019; Xiao et al., 2019; Zan et al., 2023). Numerous studies using nano-indentation have shown that the hardness increases when the indenter moves closer to a crystalline interface. Such hardening was documented in an Fe-Si bicrystal (Soifer et al., 2002). A similar observation was reported in a high-purity copper (Soer et al., 2005). In a high-purity molybdenum tricrystal, it was further observed

that the local hardening was more pronounced near triple junctions than near individual grain boundaries (Eliash et al., 2008). The same study also noted that the height of the material displaced around the indenter was lower near grain boundaries, indicating changes in the local plastic flow near the crystalline interface.

The mapping of intragranular heterogeneity of crystal orientations, as measured by Electron Backscatter Diffraction (EBSD), provides indirect insights into the plastic deformation field. Indeed, when plasticity is achieved by dislocation glide, crystal lattices reorient in response to the plastic deformation they experience (Delannay et al., 2001). EBSD is widely used when the micro-scale plastic behavior is investigated. Kernel Average Misorientation (KAM) may be derived from the EBSD maps (Pokharel et al., 2015). Indeed, this metric quantifies the average misorientation between a point in a crystal lattice and the neighboring pixels surrounding it. It has been observed that its values correlate with proximity to crystalline interfaces, with higher KAM near interfaces compared to grain centers. This phenomenon has been noted in various materials, including aluminum-magnesium alloys (Pai et al., 2022), highly annealed pure copper (Subedi et al., 2015), recrystallized commercial AA1050 sheets (Mishra et al., 2009), austenitic stainless steel (Kamaya, 2012), and aluminum-magnesium alloys (Wang et al., 2001). Another metric that can be derived from EBSD measurements is the Geometrically Necessary Dislocations density (GNDD). This type of dislocation ensures strain compatibility across grain boundaries. Using Nye's tensor, the GNDD may be estimated based on the lattice curvature measured with EBSD. In a study on DP590 dual-phase steel, the distribution of GNDs was correlated with the distance to crystalline interfaces, with the highest density located around grain boundaries (Kundu and Field, 2016). Similar results were reported in pure polycrystalline copper foils, identifying triple junctions as preferential sites for high GNDD (Jiang et al., 2013). In ferritic single-phase interstitial-free (IF) steel, higher KAM and GNDD values were also measured near interfaces compared to grain centres (Allain-Bonasso et al., 2012).

Characterizations of slip traces on surfaces have shown that slip activity varies between the center of grains and grain boundaries. These characterizations were performed on 99.999% purity bi/tricrystals copper (Wang et al., 2001), pure polycrystalline copper (Phung et al., 2014), 99.994% purity columnar-grained nickel (Li et al., 2019), polycrystalline nickel base superalloy Inconel 718 (Charpagne et al., 2021; Hestroffer et al., 2023). 3D-EBSD was used in Al-Li (2.5 wt% Li) binary alloy to extend this characterization from two dimensions to three, confirming previous observations e.g. triple junctions exhibited important values of KAM and lattice curvature (Gustafson et al.,

2023).

Numerical crystal plasticity (CP) models were used to deepen the understanding of microscopic fields. Full-field models, as Crystal Plasticity Finite Element Method (Delaire et al., 2000) or Crystal Plasticity spectral solvers (Lebensohn, 2001), can predict the distribution of microscopic fields within the microstructure. CPFEM was used to simulate a channel die experiment on pure aluminium with columnar grains (Raabe et al., 2001). They looked qualitatively at the distribution of the Taylor Factor within the microstructure, which is indicative of the local slip activity. The results showed a significant variation in the vicinity of grain boundaries, with even more pronounced changes near triple points. Similarly, a 2D simulation of the plastic compression of an aluminium polycrystal composed of columnar coarse grains in a channel die was conducted (Sachtleber et al., 2002). Their findings highlighted that triple points and grain boundaries are preferential sites for strain localization. CPFEM simulations were also used with material properties of INCO600 to investigate the distribution of equivalent total strain (elastic and plastic) relative to the distance from grain boundaries (Barbe et al., 2003). Their results showed that the average equivalent strain was uncorrelated with shortest distance to the crystalline interface. However, consistent with experimental observations in (Martin et al., 2014), they noted that the range of variation in equivalent strain was correlated with the distance to grain boundaries. Crystal plasticity mean-field models are also used to predict plastic response at the micro-scale while relying on several simplifying assumptions, which reduce computational cost. Among the most widely used are the Taylor FC (Taylor, 1938), Taylor RC (Van Houtte, 1982), self-consistent models (Lebensohn and Tomé, 1993), GIA (Crumbach et al., 2001) and ALAMEL model (Van Houtte et al., 2005). These models are effective in predicting macroscopic texture evolution and anisotropic behaviour. However, by assuming uniform deformation within each grain, they are inherently limited in their ability to capture intragranular heterogeneities in strain fields.

5.2 Characterization of microscopic heterogeneity

In this study, we aimed to characterize the microscopic heterogeneity throughout the polycrystal and assess whether there is a correlation with the proximity to crystalline interfaces, including grain boundaries, triple junctions, and quadruple points. Three characteristic distances were considered for this analysis. The first, denoted as d_{GB} , represents the distance from a point within the crystal to the nearest grain boundary, defined as the interface separating two adjacent grains. The second, d_{TL} , represents the distance to the closest triple line, formed by the intersection of three grains. Finally, the distance to

the nearest quadruple point, d_{QP} , was evaluated where a quadruple point is defined as the intersection of four grains at a single point. For the Voronoï-tessellated microstructures considered in this study, the spatial loci of points at equal distances from these interfaces exhibit characteristic geometries: points equidistant from a grain boundary define a plane, those equidistant from a triple line form a cylindrical tube, and points equidistant from a quadruple point lie on the surface of a sphere. These three types of distances are illustrated in Figure 5.1.

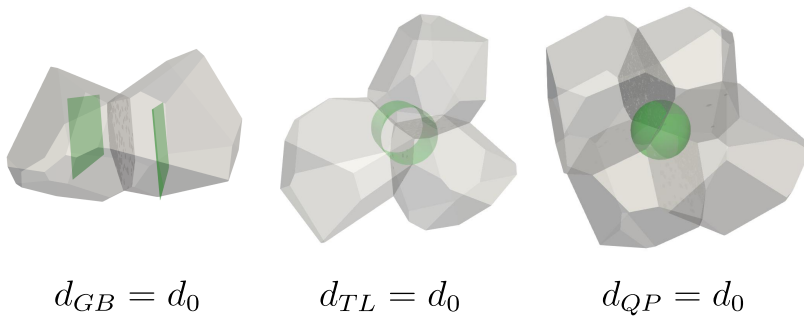


Figure 5.1: Illustration of various loci at equal distances d_0 from, respectively, the grain boundary, triple line and quadruple point.

To evaluate the influence of each type of crystalline interface, integration points of the finite element mesh were assigned hierarchically based on their proximity: first to quadruple points, then to triple lines, followed by grain boundaries, and finally to the bulk. Specifically, an integration point was considered close to a quadruple point if $d_{QP} < 0.2R$, where R denotes the average grain radius, and such points were excluded from the sets defined by $d_{TL} < 0.2R$ and $d_{GB} < 0.2R$.

5.2.1 Do crystalline interfaces influence the slip system activity?

Our CPFEM predictions indicated that the magnitude of slip activity is strongly influenced by the proximity to crystalline interfaces, with higher activity occurring in their immediate vicinity. To demonstrate this assertion, it is first necessary to explore in more detail the CPFEM constitutive model used. Here, plastic behavior was considered to be primarily governed by dislocation slip. Based on this hypothesis, the classical crystal plasticity laws were implemented in a homemade user subroutine UMAT in the commercial finite element code Abaqus/Standard (see Delannay et al. (2006) for more details). It relied on the multiplicative decomposition of the deformation gradient tensor $\mathbf{F} = \mathbf{R}^* \mathbf{U}_e \mathbf{F}_p$,

where $\mathbf{R}^*$ represents the lattice rotation tensor, $\mathbf{U}_{el}$ is the tensor related to the elastic stretch and $\mathbf{F}_p$ is deformation gradient tensor due to plastic deformation. The corresponding velocity gradient is:

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\mathbf{R}}^*\mathbf{R}^{*T} + \mathbf{R}^* (\dot{\mathbf{U}}_{el}\mathbf{U}_{el}^{-1}) \mathbf{R}^{*T} + \mathbf{R}^*\mathbf{U}_{el} \left(\dot{\mathbf{F}}_p\mathbf{F}_p^{-1} \right) \mathbf{U}_{el}^{-1}\mathbf{R}^{*T} \quad (5.1)$$

The symmetrical part of the velocity gradient $\mathbf{L}$ is the strain rate tensor $\mathbf{D}$. A viscoplastic power law was used to relate the dislocation slip rates on the slip plane α to the resolved shear stresses required to initiate dislocation motion on this plane (Hutchinson, 1977):

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{\tau_{c,\alpha}} \right|^{1/m} \text{sign}(\tau_{c,\alpha}) \quad (5.2)$$

Where $\dot{\gamma}^\alpha$ was the dislocation slip rates on the slip plane α , τ^α denotes the shear stress applied to the slip plane α , $\tau_{c,\alpha}$ was the critical resolved shear stress to trigger dislocation slip on the slip plane α and m a sensitivity exponent. Note that, in classical constitutive model, the term $\dot{\mathbf{F}}_p\mathbf{F}_p^{-1}$ corresponds to the plastic velocity gradient tensor $\mathbf{L}_p$. The components of this tensor, at a given integration point, result from the sum of shear rates:

$$\mathbf{L}_p = \dot{\mathbf{F}}_p\mathbf{F}_p^{-1} = \sum_{\alpha} \dot{\gamma}^\alpha \mathbf{b}^\alpha \otimes \mathbf{n}^\alpha \quad (5.3)$$

Where $\mathbf{n}^\alpha$ was the normal to the slip plane α and $\mathbf{b}^\alpha$ was the slip direction. A Swift hardening law was selected to model the hardening:

$$\tau_c = \tau_{c0} \left(1 + \frac{\Gamma_{tot}}{\Gamma_0} \right)^n, \quad \Gamma_{tot} = \int_0^t \sum_{\alpha} |\dot{\gamma}^\alpha| dt \quad (5.4)$$

In this formulation τ_{c0} , Γ_0 and n are material parameters. This expression enabled to link the evolution of $\dot{\gamma}^\alpha$ with $\tau_{c,\alpha}$. Here, we made the assumption that a uniform critical resolved shear stress was assigned to all slip systems. The values of $\dot{\gamma}^\alpha$ were obtained by minimizing the deformation energy which considered implicitly the hardening.

Each grain was characterized as a face-centered cubic (FCC) crystal, with dislocation glide occurring on the $\{111\} \langle 110 \rangle$ slip systems. The material properties associated with the elastic-plastic behaviour were selected based on those typically observed in commercially pure aluminium. These properties are listed in Table 5.1.

Crystal lattice	C_{11}	C_{12}	C_{44}	τ_{c0}	Γ_0	n	m	$\dot{\gamma}_0$	nr of slip plans
FCC	107.3	60.9	28.3	23	0.05	0.2	100	0.01	12

Table 5.1: Material parameters used in the constitutive model.

Different samplings of orientations were used to repeat each simulation five times, thereby eliminating any stochastic variation. All elements enclosed within the same grain boundary were assigned the same crystallographic orientation.

This study used a microstructure made of 27 grains. The geometry of the microstructure was generated using gmsh and its Vorometal plugin (Geuzaine and Remacle, 2009). It created a periodic Voronoi tessellation starting from a list of seeds provided as input (Kowalski et al., 2016). The seed positions were uniformly distributed within a cubic domain of dimension $1 \times 1 \times 1$ to obtain grains of similar sizes. The geometry was represented by a refined periodic mesh made of 37866 elements (~ 1402 el/grain) and 58510 nodes. Quadratic ten-node tetrahedral element (C3D10) were used. Both of the geometry and mesh were periodic. This periodicity of the structure eased the implementation of periodic boundary conditions (PBC) to each pair of nodes situated on opposite faces of the geometry. Further details concerning the implementation of PBCs are available in Appendix F. Additional boundary conditions were applied to dictate the macroscopic displacement of the external surfaces of the geometry. They were chosen to replicate uniaxial tension.

Using the same critical resolved shear stress, $\tau_{c0,\alpha}$ for all slip systems facilitated the derivation of a key metric: the Taylor factor, denoted as M . During plastic deformation, the microscopic plastic work is equal to the cumulative work performed by dislocation motion on all active slip systems. This balance can be expressed as:

$$\sigma_{eq} D_{eq} = \sum_{\alpha} \tau_c |\dot{\gamma}^{\alpha}| = \tau_c \sum_{\alpha} |\dot{\gamma}^{\alpha}| \quad (5.5)$$

This leads to the expression of the Taylor factor:

$$\frac{\sigma_{eq}}{\tau_c} = \frac{\sum_{\alpha} |\dot{\gamma}^{\alpha}|}{D_{eq}} = M \quad (5.6)$$

The metric M links the cumulative shear rate resulting from dislocation slip and the local equivalent strain rate. It can be interpreted not only as a measure of slip activity but also as an indicator of the local strength, and therefore of the micro-hardness, which can be probed experimentally. Therefore, the spatial distribution of M within a grain was analysed, as illustrated in Figure 5.2.

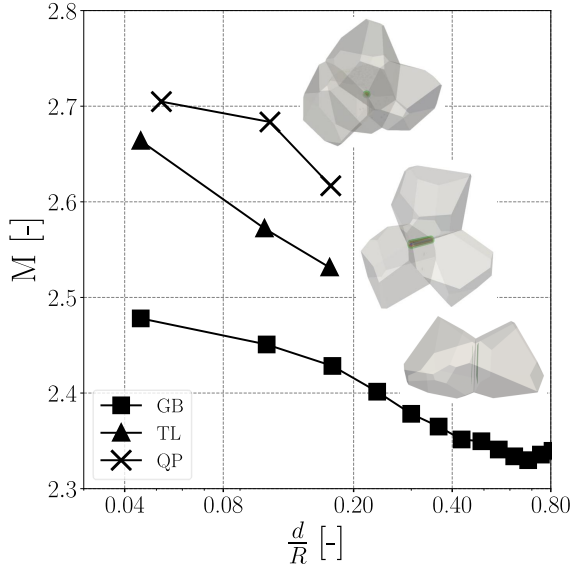


Figure 5.2: Taylor factor relative to the distance normalized by the average grain radius, for the three types of crystalline interfaces.

The magnitude of the Taylor factor was found to correlate strongly with the distance to the three types of crystalline interfaces considered. It reaches its lowest values at grain centers and increases monotonically as the distance to grain boundaries (GB), triple lines (TL), or quadruple points (QP) decreases. Regions located near these interfaces therefore require greater slip activity and higher local stresses to sustain plastic flow. These trends are consistent with numerous experimental observations reporting enhanced slip activity (elevated GND densities, higher KAM values, intensified slip traces) as well as increased hardness near crystalline interfaces. Moreover, QP and TL exhibit systematically larger Taylor factors than regions near GB, in agreement with experimental findings indicating that slip activity and hardness are generally higher in the vicinity of triple junctions than at grain boundaries (Eliash et al., 2008; Jiang et al., 2013; Gustafson et al., 2023).

5.2.2 Does the heterogeneity of plastic deformation depend on the distance to crystalline interfaces?

The combination of the intrinsic crystallographic anisotropy of individual grains and the presence of grain boundaries leads to a pronounced heterogeneity in the local strain-rate distribution within the microstructure. Indeed, in the vicinity of crystalline interfaces, some regions exhibit limited deformation while others experience comparatively high levels of strain. Nevertheless, on

average, the deformation amplitude does not appear to depend on the distance to the crystalline interface. To verify this observation, the local equivalent strain rate was analysed.

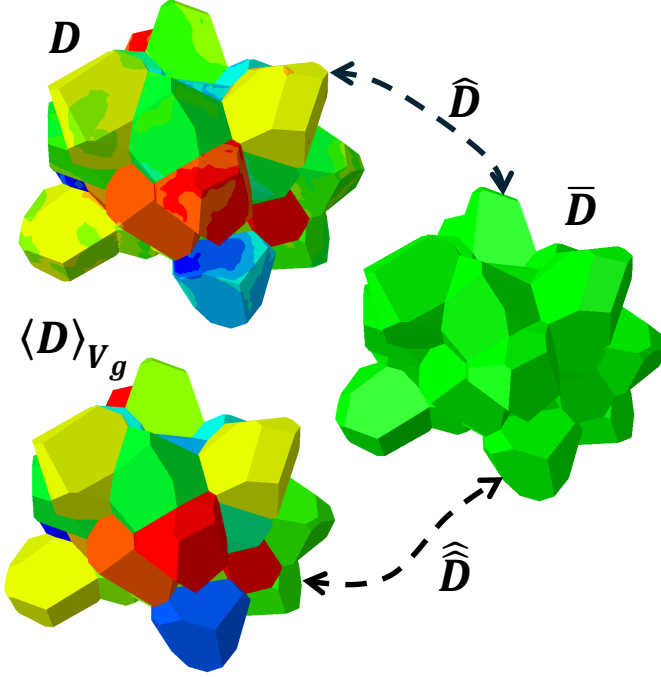


Figure 5.3: Definition of the quantities used to characterise the microscopic strain-rate field. D refers to the local strain-rate tensor, $\bar{D}$ to the macroscopic strain-rate tensor, and $\langle D \rangle_V$ to the strain rate averaged over a given volume V . The quantity $\hat{D} = D - \bar{D}$ represents the heterogeneity between the local and macroscopic strain-rate tensors, while $\hat{\hat{D}} = \langle D \rangle_V - \bar{D}$ denotes the heterogeneity between the volume-averaged and macroscopic values. For illustration purposes, the averaging volume V used to compute $\langle D \rangle_V$ has been taken equal to the volume of a grain in this example, i.e. $V = V_g$.

This local quantity is defined at each integration point as: $D_{eq} = \sqrt{\frac{2}{3} D : D}$. It was then normalized by the macroscopic equivalent strain rate, $\bar{D}_{eq}$, to identify regions where deformation is particularly significant. This analysis aimed to determine whether spatial variations in $D_{eq}/\bar{D}_{eq}$ correlated with the location relative to a crystalline interface. In Figure 5.4a, the black dots illustrate the distribution of the average value. The red and blue dots represent the distribution of the average equivalent plastic strain rates for the top 10% and bottom 10% outliers, respectively. The average equivalent strain rate remains approximately constant, with a value close to 1, throughout the grain and

shows no noticeable dependence on the distance to the considered interface. The behaviour of the outliers follows the same overall trend. This confirms that the mean local equivalent strain rate is essentially identical to the imposed macroscopic value. These findings are consistent with DIC-based experimental measurements of the equivalent strain as a function of the distance to the nearest grain boundary, thereby supporting the validity of the present predictions (Sinclair et al., 2014). The difference of approximately 0.5 between the mean (black) and the outliers (blue/red) reflects a substantial spread in the local values, indicative of pronounced intragranular heterogeneity, as also illustrated in Figure 5.4a. This constant broad distribution shows that, on average, no specific region within the grain undergoes markedly higher equivalent strain than the others. However, this apparent spatial uniformity masks an important feature: the range of variation in $D_{eq}/\bar{D}_{eq}$ increases significantly as the distance to crystalline interfaces decreases, and the largest strain-rate values are consistently located in front of an interface. These trends are fully consistent with numerous EBSD–DIC studies reporting an increase in the amplitude of local strain fluctuations near grain boundaries and other interfaces. This behaviour is clearly visible in the raw datasets provided in Appendix G.

However, the near-equivalence of the local and macroscopic equivalent strain rates ($D_{eq} \approx \bar{D}_{eq}$) did not imply kinematic similarity between the locally averaged strain-rate tensor $\mathbf{D}$ and the macroscopic strain-rate tensor, $\bar{\mathbf{D}}$. To investigate this aspect, we analysed how different the local strain-rate tensor was from its macroscopic counterpart and, thus, sought to determine whether any region within a grain exhibits deformation modes close to those imposed at the macroscopic level. For this purpose, a strain-rate heterogeneity metric was introduced and defined as: $\hat{\mathbf{D}} = \mathbf{D} - \bar{\mathbf{D}}$. The definition of this metric is illustrated in Figure 5.3. Figure 5.4b shows the evolution of the average norm of $\hat{\mathbf{D}}$ as a function of the distance to the interface. The black dots denote the mean value, whereas the red and blue symbols represent the top and bottom 10% of the data, respectively. The average value was constant at approximately 0.55 over the entire range of distances to the interface. Similarly, the outliers show no notable variation and do not display any correlation with the proximity to the interfaces. This indicates that, on average, no point within a grain developed a local strain-rate tensor that closely resembled the macroscopic strain-rate tensor, with a deviation of about 55% regardless of the distance to, or the type of, crystalline interface.

5.2.3 How do adjacent grains interact across crystalline interfaces?

In the vicinity of crystalline interfaces, the deformation of individual grains is restricted by the neighbouring grains, as overall compatibility must be main-

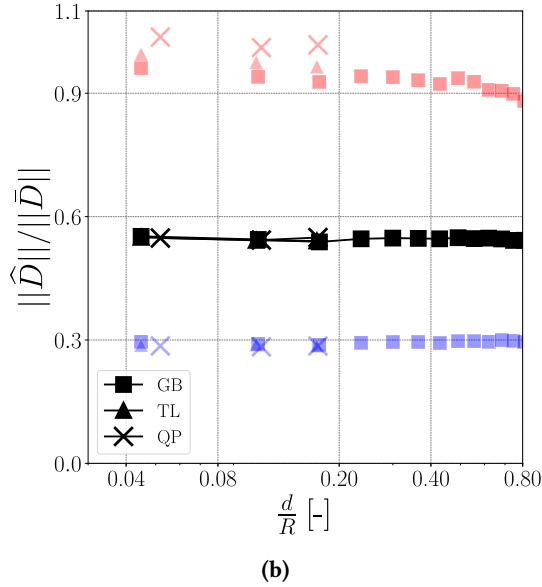
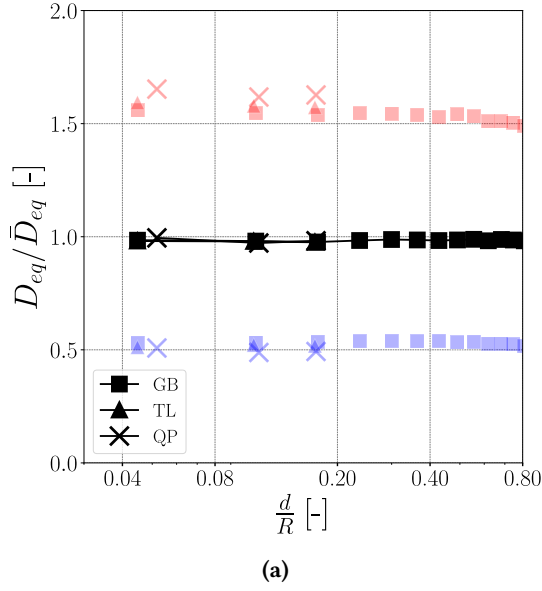


Figure 5.4: Distribution of (a) the equivalent strain rate D_{eq} and (b) the heterogeneity of the local strain rate $\hat{D}$ as a function of the normalised distance to the grain boundary (GB), triple line (TL) and quadruple point (QP). The distance is normalised by the average grain radius. Black dots denote the average values, while blue and red symbols correspond to the lowest and highest 10% of the data, respectively.

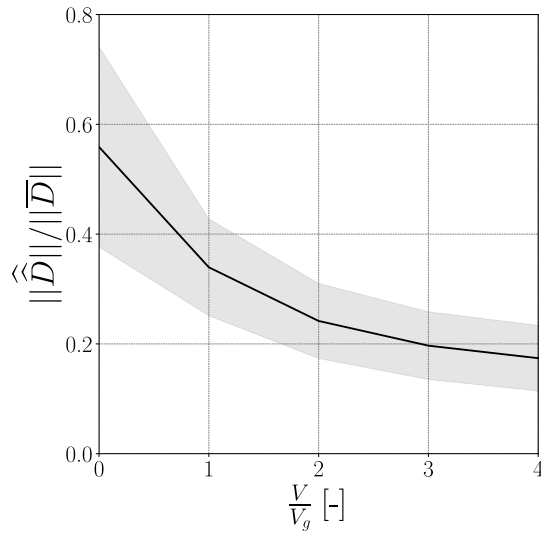
tained. In this study, we show that the deformation of a volume covering grain boundaries are more closely aligned with the macroscopic strain and that the strain difference across the grain boundary corresponded mainly to opposite shear deformations. In order to verify it, we calculated the norm of the tensor $\widehat{\widehat{D}}$, defined as $\widehat{\widehat{D}} = \langle D \rangle_V - \bar{D}$. The tensor $\widehat{\widehat{D}}$ is analogous to the previously defined tensor $\widehat{D}$, except that it compares the volume-averaged strain rate over a domain V with the macroscopic strain rate.

In Figure 5.5a, the solid line shows the evolution of this metric for a region increasing in volume, constructed by sequentially adding randomly selected integration points of the FE mesh, each contributing a small surrounding volume. This eliminates any bias related to the initial position. The grey band surrounding the line represents the standard deviation. This random procedure was repeated five times, and the black line corresponds to the mean value of these five realisations. Both the mean value and the standard deviation decrease monotonically when increasing number of integration points considered. As a result, the strain-rate heterogeneity gradually diminishes and tends towards 0 as all integration points are included. The values of this metric for equivalent volumes of one, two, and three grains are listed in Table 5.2.

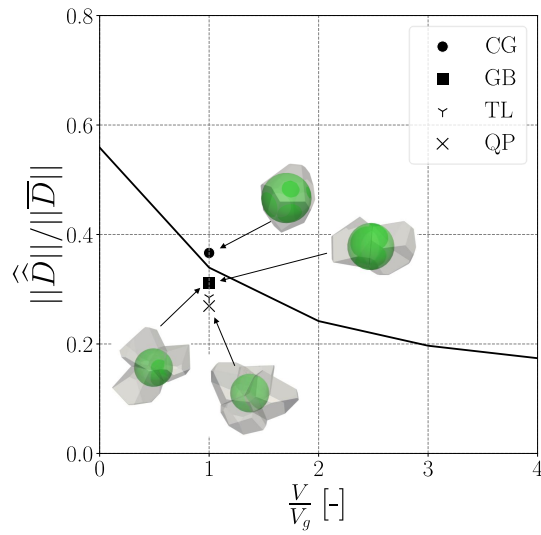
We then evaluated the evolution of the norm of strain rate heterogeneity $\widehat{\widehat{D}}$ for spherical volumes having an average grain volume. These spheres were positioned at different types of crystalline interfaces as well as at the grain centres. The data points shown in Figure 5.5b represent average values obtained for all spheres located at a given type of location. Values below the black curve indicate that the region deforms more closely to the macroscopic strain rate than a randomly selected volume of the same size. This is observed for all spheres positioned at crystalline interfaces. The only value above the black curve corresponds to the grain centre. Among the interface locations, the smallest deviation occurs at the quadruple points (QP), followed by the triple lines (TL), and finally the grain boundaries. The corresponding values are listed in Table 5.2.

	1 grain	CG	2 grains	GB	3 grains	TL	4 grains	QP
$\frac{\ \widehat{\widehat{D}}\ }{\ \bar{D}\ }$	0.36	0.37	0.24	0.31	0.19	0.28	0.15	0.27

Table 5.2: Comparison of the magnitude of the equivalent strain rate heterogeneity, $\widehat{\widehat{D}}_{eq}$, between a randomly selected volume corresponding to n grains and a spherical volume equivalent to a single grain, positioned at the Center of Grain (CG), Grain Boundary (GB), Triple Line (TL), and Quadruple Point (QP).



(a)



(b)

Figure 5.5: Evolution of (a) the magnitude of strain rate heterogeneity, $\|\hat{\bar{D}}\|$, within a randomly selected volume V , and (b) the magnitude of strain rate heterogeneity within a spherical volume V located near crystalline interfaces and near grain centers. The volume V was normalized by the average volume of 1 grain V_g .

It is important to emphasise that the deformation of a crystalline interface involving the intersection of n grains cannot be regarded as equivalent to the deformation of n independent grains. Indeed, the data in Table 5.2 showed that, for spherical volumes having the size of 1 grain and located at grain boundaries, triple lines or quadruple points, the strain-rate deviation is consistently higher than that of a volume covering 2, 3 or 4 grains. Moreover, this difference increased with the number of intersecting grains. This observation can be attributed to the fact that a volume composed of n randomly selected grains reflects, on average, a deformation corresponding statistically to a region n times larger than the virtual sphere used in the present analysis. Consequently, such larger volume converges more rapidly towards the macroscopic strain rate.

Since the total deformation within each spherical volume resulted from the combined contribution of the individual grains it contained, we further examined how the deformation differed between these grains. This analysis was restricted to the cases involving grain boundaries, i.e. not the QP and TL regions. To this end, we introduced a metric, denoted by λ , which quantified the fraction of the strain heterogeneity that is attributable to shear parallel to the grain boundary. This parameter is expressed as:

$$\lambda = \frac{\sqrt{2 (\Delta D_{13}^2 + \Delta D_{23}^2)}}{\sqrt{\Delta D_{11}^2 + \Delta D_{22}^2 + \Delta D_{33}^2 + 2 (\Delta D_{12}^2 + \Delta D_{13}^2 + \Delta D_{23}^2)}} \quad (5.7)$$

where ΔD_{ij} corresponds to the difference between the ij component of the strain rate tensor computed for each half-sphere, expressed in a local coordinate system in which the axis normal to the separating grain boundary is $\mathbf{e}_3$. Consequently, a value of λ^2 approaching unity indicates that the local strain difference across the grain boundary is dominated by shear deformation parallel to the interface. The ideal case of $\lambda^2 = 1$ is shown in Figure 5.6. Details concerning the derivation of λ are provided in the Appendix H. The spherical volume was restricted to $V_g/10$ in order to minimise the influence of neighbouring crystalline interfaces.

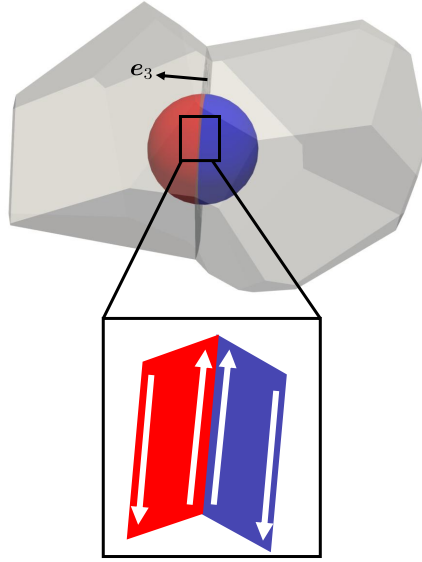


Figure 5.6: Illustration of the ideal case $\lambda^2 = 1$, where deformation heterogeneity between neighbouring grains corresponds to opposite shear parallel to the grain boundary.

Figure 5.7 confirms the main hypothesis of the ALAMEL model, according to which the deformation heterogeneity between two grains is largely governed by opposite shear, as indicated by the relatively high value of λ^2 , particularly for the smallest considered volume. For the smallest virtual sphere, representing less than 1% of the average grain volume, the metric takes a value of approximately 0.79. Taking into account the associated standard deviation gives $0.55 < \lambda^2 < 1$. As the volume of the sphere increases, λ^2 steadily approaches 0.5. This can be attributed to the fact that larger volumes include the influence of additional crystalline interfaces. Hence, the main source of deformation heterogeneity between interacting grains can be attributed to opposite shear deformation.

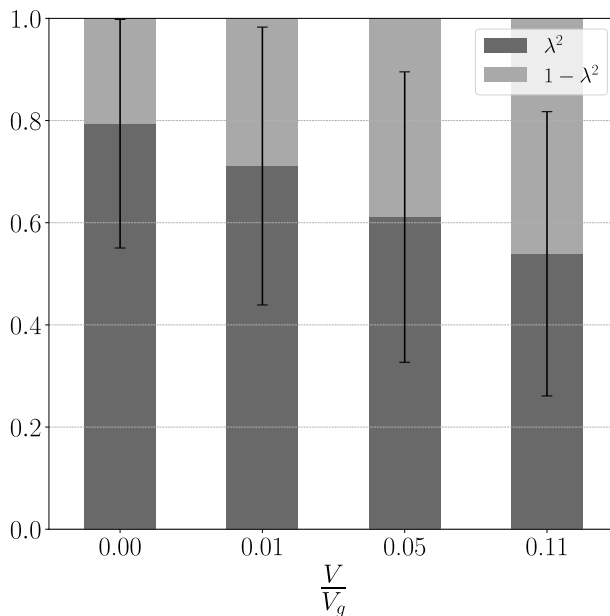


Figure 5.7: Magnitude of the metric λ^2 for spherical volumes, located on grain boundaries, for different normalised volume.

5.3 Capturing crystalline interface heterogeneity in non-conformal FE

As illustrated in Figure 5.8, when the finite element mesh does not conform to the grain boundaries, different situations are encountered. Some finite elements are entirely contained within the core of a single grain but others, however, are intersected by crystalline interfaces, such as grain boundaries or triple junctions. Elements intersected by interfaces present a particular challenge: if all integration points within an element are assigned the same crystallographic orientation, the proximity of crystalline interfaces and their influence on local strain heterogeneity are neglected, potentially underestimating deformation gradients in these regions.

In the proposed simplified CPFEM framework adapted to non-conformal meshes, interactions with adjacent grains are accounted for at the level of individual integration points. The treatment of each point depends on its distance to the nearest interface. To this end, the three nearest grain centroids, labelled a , b and c , are identified in the Voronoï tessellation, with the studied integration point belonging to the Voronoï cell a . The shortest distances to the grain boundaries separating the host grain and its neighbours, $\{d_{ab}, d_{ac}\}$ are also computed according to the procedure detailed in Appendix I. These distances are compared to a characteristic length, noted l_c , which corresponds

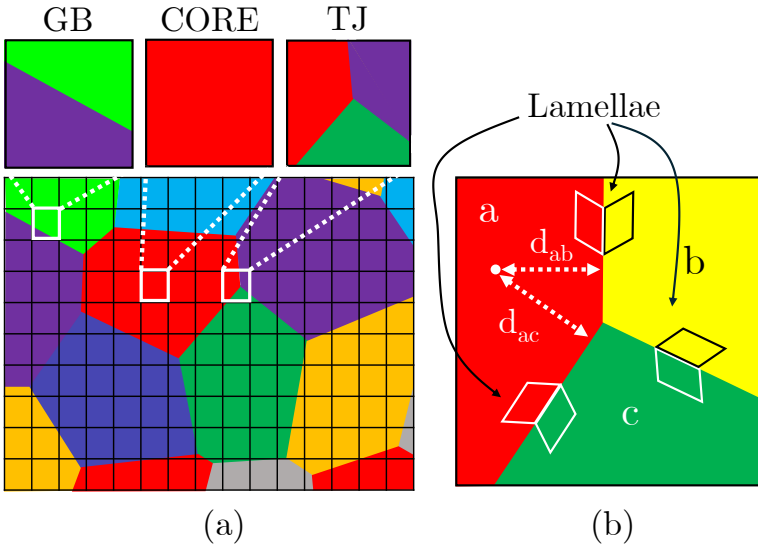


Figure 5.8: (a) Inside a non-conforming mesh, integration points can belong either to CORE element or to grain boundary (GB) element or triple junction (TJ) element. (b) Definition of the distances d_{ab} and d_{ac} to the nearest crystalline interfaces. Grain a denotes the host grain, while grains b and c represent nearby adjacent grains. The three lamellae modelling the grain interactions are also presented.

the maximum distance from a grain boundary over which the interaction with neighbouring grains is considered.

As illustrated in Figure 5.9, the stress tensor predicted at an integration point may have either only one or several contributions:

1. CORE configuration: the integration point lies well within the core of grain a , it is unaffected by interactions with the neighbouring grains ($d_{ab} > l_c$). The classical single-crystal CPFEM formulation is applied.
2. Grain boundary (GB) configuration: if the integration point is close to a single grain boundary ($d_{ab} < l_c$ and $d_{ac} > l_c$). The local stress is computed as a weighted sum of the stress in grain a and the stress inside a lamella representing the interaction with grain b .
3. Triple junction (TJ) configuration: if the integration point is close to two grain boundaries ($d_{ab} < l_c$ and $d_{ac} < l_c$). Three lamellae are therefore considered to account for interactions between the grain pairs (a, b) , (a, c) and (b, c) , in addition to the stress predicted in the host grain a .

Each contribution is thus weighted according to the distance of the integration point to the corresponding grain boundary: the lamella weight decreases with increasing distance from the boundary, whereas the residual single-crystal weight gains increases. Regardless of the configuration, the sum of the weights is always equal to 1. At each time increment, the same deformation gradient F is applied to all sub-regions, which each contribute to the stress tensor. Their weighted contributions define the local stress state. It should be noted that quadruple points are not explicitly treated here, due to their low occurrence relative to grain boundaries and triple junctions.

The interaction inside a lamella is modelled using an approach analogous to the ALAMEL model, which has demonstrated excellent performance in predicting texture evolution and macroscopic plastic anisotropy (Van Houtte et al., 2005). Accordingly, the velocity gradients of the two interacting grains are expressed as:

$$\begin{aligned} L^I &= \dot{F} F^{-1} + \dot{\gamma}_{rlx}^{(1)} (\mathbf{p}^1 \otimes \mathbf{n}) + \dot{\gamma}_{rlx}^{(2)} (\mathbf{p}^2 \otimes \mathbf{n}) \\ L^{II} &= \dot{F} F^{-1} - \dot{\gamma}_{rlx}^{(1)} (\mathbf{p}^1 \otimes \mathbf{n}) - \dot{\gamma}_{rlx}^{(2)} (\mathbf{p}^2 \otimes \mathbf{n}) \end{aligned} \quad (5.8)$$

Here, F is the deformation gradient of the lamella (identical to that imposed on each contribution), L^I and L^{II} denote the velocity gradients of grains I and II , $\mathbf{p}^1$ and $\mathbf{p}^2$ are directions parallel to the grain boundary plane, $\mathbf{n}$ is the normal to this plane, and $\dot{\gamma}_{rlx}^{(1)}$ & $\dot{\gamma}_{rlx}^{(2)}$ are the associated relaxation shear rates along $\mathbf{p}^1$ and $\mathbf{p}^2$. These relaxation introduce additional degrees of freedom that lower the local deformation energy while maintaining compatibility with the

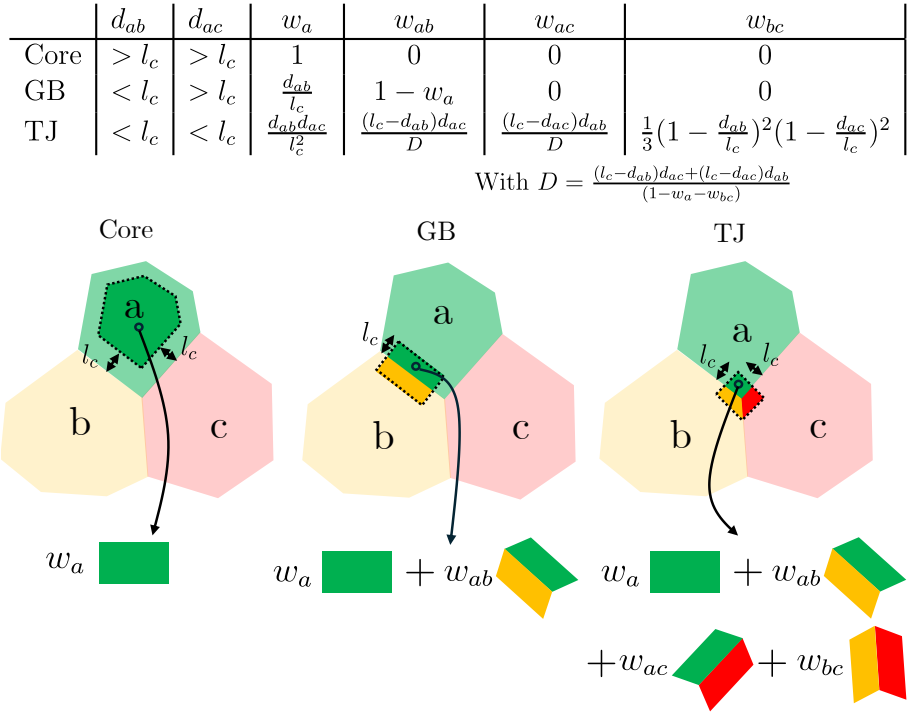


Figure 5.9: Definition of the weights associated with the different interactions influencing to the prediction of the strain field at a given integration point. The values of these weights depend on the distances to the nearest grain boundaries, d_{ab} and d_{ac} , as defined in Figure 5.8(b).

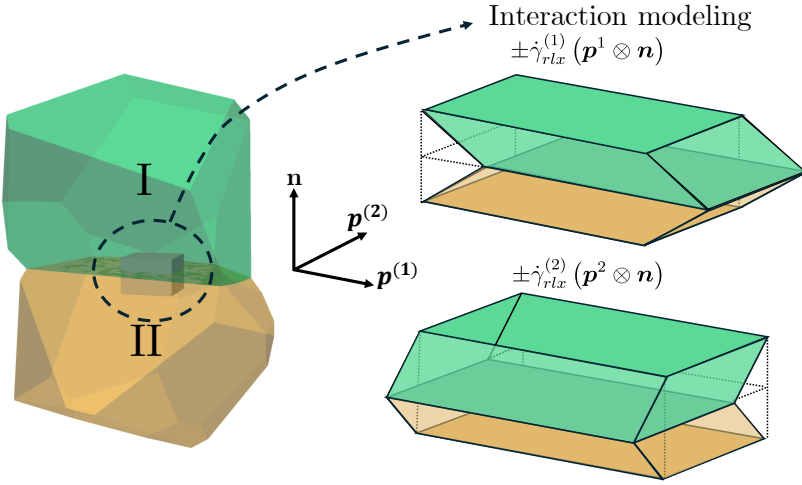


Figure 5.10: The interaction between two grains is modelled using a lamella, in which the local strain heterogeneity corresponds to opposite shear rates ($\dot{\gamma}_{rlx}$) parallel to the grain boundary with normal vector n .

imposed macroscopic strain. Their magnitudes are determined simultaneously with the dislocation slip rates through an energy minimization procedure (Delannay et al., 2009). The implementation was verified through a series of consistency and sanity checks. Details of these validation procedures are provided in Appendix J.

This extended formulation was implemented inside a UMAT subroutine.

The efficiency of the novel CPFEM framework to improve the accuracy of simulations performed on non-conformal meshes was assessed based on a comparison with reference CPFEM simulations.

Non-conformal meshes used eight-node brick-shaped elements (C3D8) of Abaqus. Two levels of mesh refinement were considered, consisting of 125 and 1000 elements (Figure 5.11). In such coarse mesh, a significant proportion of elements are intersected by grain boundaries or triple junctions, as shown in Table 5.3. Two types of simulations were performed:

- Standard approach: each element was assigned a single crystallographic orientation, corresponding to the Voronoï cell hosting the largest fraction of the element volume.
- Novel approach: the proximity of crystalline interfaces was accounted by using lamellae. The characteristic length parameter l_c was related to the mesh discretization and scaled as $l_c \propto \vartheta \left(\frac{dim}{n} \right)$, where dim is the domain edge length (equal to 1 in this study) and n is the number of

	# elem.	# nodes	CORE	GB	TJ
Non-conformal mesh (a)	125	216	13.6%	24.8%	61.6%
Non-conformal mesh (b)	1000	1331	45.4%	32.5%	22.1%
Conformal mesh (c)	6296	10669	100%	0%	0%
Conformal mesh (d)	14352	23338	100%	0%	0%
Conformal mesh (e)	27561	43276	100%	0%	0%
Conformal mesh - ref (f)	37866	58510	100%	0%	0%

Table 5.3: Specifications of the different meshes. CORE refers to proportion elements located entirely within a grain, while GB and TJ denote the percentage of elements intersected by a grain boundary or a triple junction. The conformal mesh (f) corresponds to the mesh used to obtain the reference results and is identical to that employed in Part I of this study.

voxels along that edge. For instance, the mesh containing 125 elements ($5 \times 5 \times 5$) used $l_c = 0.07$, whereas the one with 1000 elements ($10 \times 10 \times 10$) used $l_c = 0.02$.

Another set of reference simulations were performed on conformal meshes which were generated with ten-node tetrahedral elements (C3D10) of Abaqus. Four refinement levels were considered as detailed in Table 5.3. In these meshes, the elements were never intersected by a crystalline interface so that all integration points could be assigned the same crystallographic orientation.

For both types of meshes, the periodic boundary conditions ensured macroscopic uniaxial tension along the x -direction. The same five sets of 27 random crystallographic orientations, as in Part 1 of this study, were tested in order to smooth out stochastic variations.

As illustrated in Figure 5.12, local accuracy of the predictions was measured at the element scale, based on the following metric:

$$\tilde{D} = \langle D \rangle_{coarse} - \langle D \rangle_{ref} \quad (5.9)$$

where $\langle D \rangle_{coarse}$ denotes the element-averaged strain rate obtained from simulations using a coarse non-conformal or conformal mesh, while $\langle D \rangle_{ref}$ corresponds to the strain rate averaged over a volume of identical shape and location in the most refined simulation using a conformal mesh.

Figure 5.13 shows the evolution of $\tilde{D}$ as a function of computational time. For both mesh types, decreasing the number of elements systematically degraded the accuracy. The lowest accuracy was obtained with the non-conformal meshes using the standard approach. Introducing the novel approach greatly improved the results: for the 125-element mesh, the accuracy

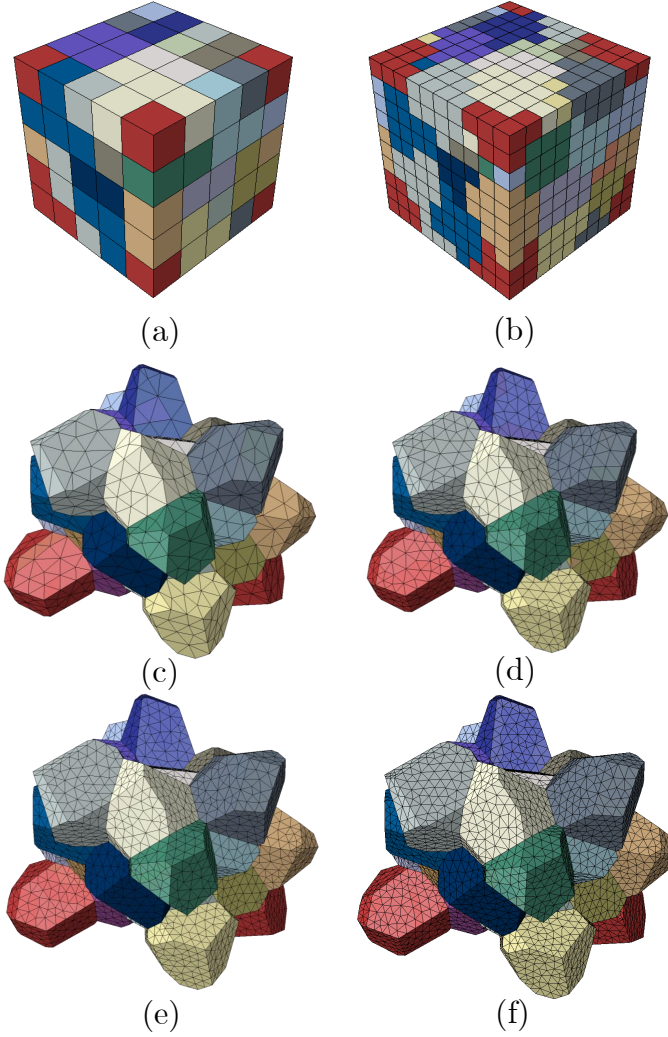


Figure 5.11: 27-grain microstructure meshed with two non-conformal meshes and 4 conformal meshes made of (a) 125 elements, (b) 1000 elements, (c) 6296 elements, (d) 14 352 elements, (e) 27561 elements and (f) 37866 elements. The conformal mesh (f) was already used in Part I of this study.

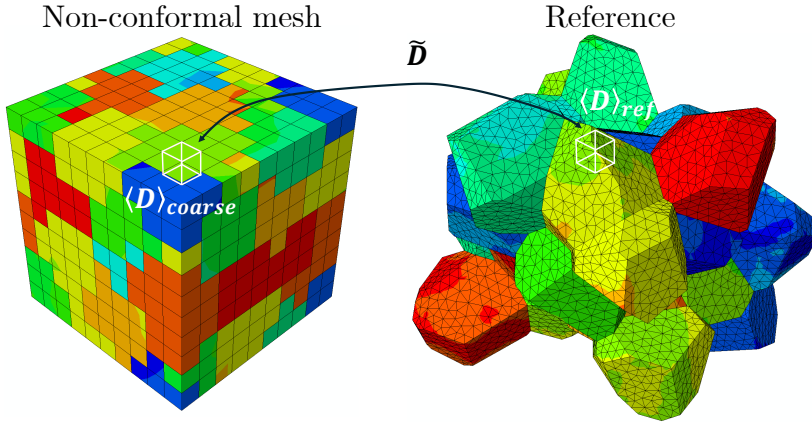


Figure 5.12: Definition of the local accuracy at the element scale. $\langle D \rangle_{coarse}$ denotes to average strain-rate tensor over a coarse mesh element, while $\langle D \rangle_{voxel,ref}$ corresponds to the average strain-rate tensor over an identically shaped and positioned volume in the reference simulation. The quantity $\tilde{D} = \langle D \rangle_{coarse} - \langle D \rangle_{ref}$ provides a measure of the local accuracy by quantifying the deviation over each element from the reference simulation.

improved from 0.24 to 0.16 and for the 1000-element mesh, from 0.18 to 0.13. These levels of accuracy are comparable to those obtained with a conformal mesh containing ~ 6000 elements.

Regarding computational efficiency, voxel-based non-conformal meshes with 125 and 1000 elements were approximately 6 and 3 times faster, respectively, than the conformal mesh with ~ 6000 elements. The new approach did not increase computational cost relative to the standard one.

The macroscopic stress–strain responses are compared in Figure 5.14. For clarity, only the results from the least and most refined conformal meshes are shown. All simulations produced similar macroscopic responses. Coarser meshes only very slightly overestimated the flow stress relative to the reference. Compared to the standard approach on non-conformal meshes, the novel approach predicted a stress that was slightly smaller, and in marginally closer agreement with the reference curve.

5.4 Discussion

The present study introduces an enhanced CPFEM framework that accounts for grain interaction across crystalline interfaces. Each interaction is represented as a lamella, following ideas borrowed from ALAMEL crystal plasticity model, originally developed to predict texture evolution in polycrystals (Van Houtte et al., 2002; Delannay et al., 2009). While the original ALAMEL model assumed

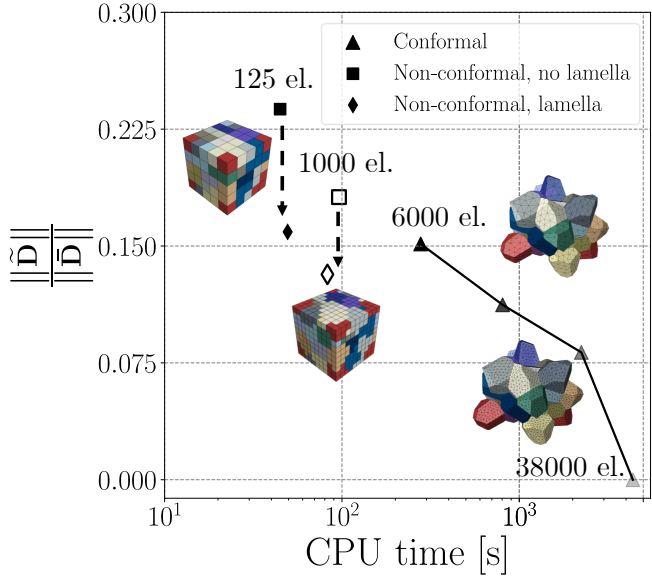


Figure 5.13: Local accuracy of the strain field as a function of the required computational time obtained from different simulations. Empty squares and diamonds correspond to non-conformal meshes composed of 1000 elements, whereas the filled symbols represent those with 125 elements. The color gradient within the triangles indicates the number of elements, with lighter shades corresponding to finer meshes.

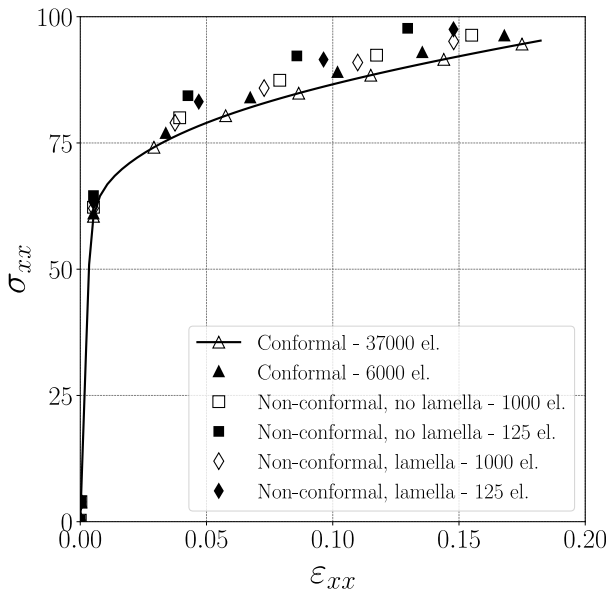


Figure 5.14: Macroscopic tensile curve predicted for different approaches: standard CPFEM with conformal mesh, standard CPFEM with non-conformal mesh, and enriched CPFEM with non-conformal mesh.

that the macroscopic strain was achieved within each lamella (Van Houtte et al., 2005), the novel CPFEM approach imposes on the lamellae a local strain derived from the finite element solution. To the authors' knowledge, this represents the first implementation within a CPFEM framework that considers the influence of interactions with neighboring grains on the prediction of the local response.

The adoption of this interaction scheme is justified by the findings presented in Part I of this study. Analysis revealed that the average deformation of spherical subdomains approximates the macroscopic strain rate more closely when these subdomains are centered on crystalline interfaces. This indicates that grains interacting across interfaces accommodate the macroscopic deformation more effectively than grains located near the center, where such interactions are absent. Furthermore, in the vicinity of these interfaces, adjacent grains deform in a manner such that the primary source of local strain heterogeneity arises predominantly from opposing shear components along the grain boundary. These observations support the use of an ALAMEL-type interaction approach, as they are consistent with the hypotheses underlying the ALAMEL model (Van Houtte et al., 2005).

However, it is important to acknowledge that the characteristics of microscopic strain heterogeneity discussed in Part I were derived exclusively from CPFEM

simulations. Consequently, rigorous experimental investigation, combining EBSD with digital image correlation (DIC) or using High-Resolution Electron Backscatter Diffraction (HR-EBSD) during in-situ deformation, is necessary to validate these numerical predictions. Furthermore, a direct comparison between the experimental deformation field and the results obtained using the novel CPFEM formulation, on a geometry reproducing the same microstructure as that used for the experimental measurements (e.g., Lin et al. (2020)), would provide a robust basis for refining the weighting schemes employed in the proposed methodology.

Moreover, it is essential to note that all the results were obtained without considering intragranular stress arising from dislocation substructures. Specifically, the current approach does not account for the development of back stresses resulting from the pile-up at grain boundaries. Since such backstresses are likely to influence deformation kinematics near the interface, incorporating these micromechanical features remains a critical avenue for future investigation.

For coarse non-conformal meshes, the proposed method substantially enhanced the accuracy of local strain predictions while preserving the low computational cost of voxelized discretizations. Specifically, non-conformal meshes with only 125 and 1000 elements achieved element-level accuracy comparable to that of a conformal mesh with approximately 6000 elements, while requiring only about 20% of its CPU time. Note that the macroscopic stress-strain predictions remained nearly identical to those obtained using the standard CPFEM formulation, which already agreed well with the reference. Consequently, this novel approach provides an attractive strategy for predicting realistic microscopic strain fields at reduced computational cost. An alternative would be to employ highly refined non-conformal meshes, as commonly done in the literature (Li et al., 2016), which limit geometric inaccuracies near interfaces but drastically increases computational cost.

Finally, the interest of this interaction framework is likely dependent on the crystalline symmetry of the material. The present study focused exclusively on FCC aggregates. In such crystals, as well as in BCC metals, the large number of available slip systems tends to mitigate strain heterogeneity compared to lower symmetry structures (Tang et al., 2019). Indeed, in Hexagonal Close-Packed (HCP) crystals, the limited number of independent slip systems and strong plastic anisotropy is known to foster severe strain heterogeneity (Bieler et al., 2009; Britton et al., 2015). Therefore, it is expected that the proposed framework will yield even greater gains in accuracy for HCP materials. Further research is required to confirm this hypothesis.

5.5 Conclusion

In this study, the heterogeneity of the microscopic deformation field inside a polycrystal was characterized within a grain and especially near crystalline interfaces, including grain boundaries (GB), triple lines (TL), and quadruple points (QP). This analysis was conducted using multiple CPFEM simulations on a microstructure discretized with a highly refined conformal mesh. The key findings are summarized as follows:

1. The Taylor factor increased, on average, as the distance to GB, TL, or QPs decreased. This effect was further amplified in regions adjacent to crystalline interfaces when the number of interacting grains increased.
2. The mean amplitude of the local equivalent plastic strain rate did not depend of the distance from crystalline interfaces, and no intragranular region exhibited larger deformation.
3. Mean deformations of spherical regions centered on GB, TL, and QP more closely approximated the macroscopic deformation of the polycrystal than regions located near grain centers.
4. Strain heterogeneity across grain boundaries was, on average, dominated by opposite shear components.

In Part 2 of this study, a novel approach for CPFEM simulations employing non-conformal meshes was introduced. In this framework, interactions between neighbouring grains are accounted for at the level of integration points, using a formulation derived from the ALAMEL model. The conclusions drawn in Part 1 of this study supported the use of an ALAMEL-type scheme for modelling grain interactions. The proposed method demonstrated excellent performance, as summarized below:

1. A significant gain in accuracy was achieved at the element scale for the predicted microscopic strain field, without compromising the precision of macroscopic quantities when using non-conformal meshes.
2. Important reduction in computational time was achieved compared to conformal meshes, providing an equivalent level of accuracy.

In this work, we sought to elucidate and predict the development of heterogeneous stress and plastic strain fields in metallic alloys at both the micro- and macroscopic scales. To this end, we exploited the strong interplay between plastic deformation and crystallographic texture. Throughout the thesis, it was demonstrated that both the initial texture (prior to deformation) and the developed texture (after processing) provide valuable source of information concerning the spatial heterogeneity of stress and strain distributions. This section presents the main scientific contributions of the thesis and proposes several perspectives for future research.

Summary of the contributions

Based on the conclusions drawn at the end of each chapter, we can now provide answers to the scientific questions that motivated this work.

How does a through-thickness texture gradient, induced by extrusion, influence the development of heterogeneous stress fields during subsequent plastic processing?

In forming analyses, macroscopic texture has primarily been used to predict the anisotropic response of sheet metals, often overlooking the spatial distribution of this texture. In Chapter 3, by coupling experimental characterization with crystal plasticity (CP) simulations, we demonstrated that the discrepancy in anisotropic response, dictated by non-uniform crystallographic textures across the thickness, is not a negligible microstructural detail, but rather a primary driver of macroscopic internal stress generation upon subsequent plastic deformation. Specifically, we established that both the magnitude and the through-thickness distribution of these internal stresses are highly dependent on the loading direction. Consequently, characterization of the texture gradient provides critical new insights for engineers in process design to preserve the structural integrity and mechanical performance of the final components. Indeed, the loading direction during subsequent forming steps must be carefully selected to mitigate the development of these stress gradients.

Furthermore, this study extends the conventional scope of CP modelling.

While primarily employed to predict texture evolution or to resolve local intergranular stress and strain, we proved that these frameworks can accurately predict macroscopic internal stress fields originating from macro-scale texture gradients. Moreover, for the case studied, we revealed that computationally efficient mean-field CP schemes are just as accurate as expensive full-field approaches in capturing both the magnitude and the spatial distribution of these stresses. These findings position mean-field models as accessible and efficient tools for evaluating macro-scale internal stresses in gradient-textured materials.

What is the strain heterogeneity across the thickness of roll-bonded multilaminates, and how can this strain gradient be revealed?

Measuring through-thickness plastic strain heterogeneity in roll-bonded multilaminates is inherently challenging due to the complex, non-uniform deformation paths experienced across the thickness. Indeed, in the Fe-Al multilayer studied in Chapter 4, we showed that deformation gradient is strongly related to the position of the different constituting phases across the thickness. The softer constituent layers (e.g., aluminium) act as strain localizers, accommodating severe plastic deformation dominated by intense shear. Conversely, the harder layers (e.g., iron) predominantly experience conventional plane strain compression near the mid-plane, while those positioned further from the center accumulate moderate shear parallel to the rolling plane. Revealing these strain gradients has traditionally relied heavily on computationally expensive finite element simulations, as utilized in this thesis, or intricate experimental methods, such as DIC and local probing techniques. While crystallographic texture has long been employed to deduce the thermomechanical history of materials, its application has largely been confined to regions exhibiting homogeneous textures - typically resulting from uniform macroscopic deformation or phase transformations. Supported by both macroscopic and crystal plasticity finite element (CPFEM) simulations on Fe-Al multilaminates, we pushed this approach further: we demonstrated that through-thickness texture gradients themselves can be exploited to probe local strain gradients. We proved the robustness of this approach even in complex multilayer systems developing unconventional deformation fields. A key strength of this methodology lies in its resilience. We demonstrated that even with the emergence of layer instabilities, the spatially averaged texture remains a reliable indicator of the average plastic strain state within a given layer.

In conclusion, this approach empowers researchers and engineers to deduce through-thickness strain heterogeneity directly from post-mortem orientation maps, providing a framework to optimize roll-bonding process parameters (preventing the emergence of interfacial instabilities and limiting the development of detrimental internal stresses).

How does proximity to crystalline interfaces affect plastic deformation, and how can these effects be incorporated into a CPFEM framework?

Characterizing the heterogeneity of microscopic deformation fields near crystalline interfaces has traditionally relied on experimentally coupling electron backscatter diffraction (EBSD) with digital image correlation (DIC). However, these measurements are inherently restricted to 2D free surfaces, impeding a comprehensive spatial characterization of the mechanical response as a function of distance from the boundary. In Chapter 5, we overcame this limitation by examining the deformation fields within 3D polycrystalline aggregates using CPFEM. We showed that the local plastic response within a grain is influenced by its proximity to a crystalline interface. Moreover, we revealed that the nature of these grain interactions near grain boundaries aligns with the assumptions underlying the ALAMEL model.

Building on these observations, a novel CPFEM framework was developed and implemented. In this formulation, interactions with adjacent grains are accounted for at the integration point level, weighted according to their distance to the nearest interface. This novel approach fundamentally relaxes conventional meshing constraints. Indeed, we demonstrated that it improves the predictive accuracy of CPFEM when utilizing computationally efficient coarse and non-conformal meshes. Consequently, it offers a pragmatic and efficient strategy for simulating the plastic deformation of polycrystalline aggregates, circumventing the prohibitive computational costs traditionally associated with highly refined, conformal meshes.

Perspectives for future research

Beyond the findings obtained in this work, several promising directions emerge for extending the present research. The most compelling of these perspectives are presented below.

Revealing heterogeneous fields in AISI 410/SS316L multilayers

It was shown that texture heterogeneity can provide valuable information about the presence of plastic strain gradients, while such non-uniformity in texture can also induce internal stresses under additional plastic deformation. These two phenomena were investigated separately in Chapters 3 and 4. They also motivate an ongoing study, which was initiated recently and did not finalize yet, in a multilayer produced by roll-bonding, consisting of alternating layers of austenitic 316L stainless steel and martensitic 410 stainless steel. Preliminary investigations, detailed in Appendices A and B, already suggested the

presence of a plastic strain gradient generated during the rolling step, as well as the potential development of significant internal stresses under subsequent plastic deformation. Further investigations should allow us to confirm these first results and strengthen the use of texture as a predictive tool to reveal and characterize heterogeneous fields across such multilayered materials.

Texture-based analysis of local plastic strain fields

The present work has demonstrated the potential of using macroscopic crystallographic texture to inform about the distribution of plastic strain within each layer of rolled multilayered materials. Building on this, it is of interest to explore the possibility of deducing local plastic strain fields from microscopic crystallographic texture. Preliminary results (Appendix C) indicate that texture can evolve even in the absence of dislocation slip, as rigid body rotations of rigid layers may produce similar signatures. Nonetheless, access to high-quality EBSD orientation maps, combined with accurate knowledge of the spatial arrangement of individual layers, opens a promising route for resolving strain gradients at finer scales.

Texture as a design lever for controlling plastic anisotropy and internal stress in architected materials

This work has shown that initial texture gradients in extruded sheets can strongly influence both macroscopic plastic anisotropy and the subsequent development of internal stresses during later forming stages. In the context of extrusion, several studies have already demonstrated the ability to control the thickness of peripheral coarse-grain (PCG) regions (Zhao et al., 2023; Negrozio et al., 2024, 2025b). As a result, PCG-related texture features may be considered as design parameters for adjusting macroscopic plastic anisotropy while simultaneously influencing internal stress evolution.

More broadly, in the design of multilayered materials, the initial texture of individual layers represents an opportunity for tailoring unconventional macroscopic plastic responses. For example, it may enable the development of nearly isotropic macroscopic behavior from intrinsically anisotropic constituents. At the same time, systematic exploration of texture combinations could provide guidelines for mitigating internal stresses arising from deformation incompatibilities between layers. Finally, texture-informed strategies could be employed to optimize stacking sequences. By anticipating which layers experience tension or compression during subsequent forming operations, engineers may avoid placing highly sensitive textures in positions that would exacerbate stress localization or promote failure, such as external layers subjected to tensile loading during bending.

Experimental investigation of the microscopic strain heterogeneity

The characteristics of microscopic strain heterogeneity presented in Chapter 5 were derived solely from CPFEM simulations. A proper experimental investigation, combining EBSD with digital image correlation (DIC) during in situ deformation, would allow these characteristics to be confirmed and provide stronger validation for the proposed approach. Furthermore, direct comparison between the experimental deformation field and the results obtained using the novel CPFEM formulation on a geometry reproducing the same microstructure as that used for the experimental measurements (Lin et al., 2020) could help refine the weighting schemes employed in the proposed methodology.

Deeper assessment of the proposed CPFEM implementation

The novel approach proposed for CPFEM simulation showed promising first results, but further investigations are required to fully exploit its potential. Firstly, the current study focused exclusively on face-centered cubic (FCC) crystals. Extending this approach to crystals with different slip system definitions, such as body-centered cubic (BCC) and hexagonal close-packed (HCP) structures, would provide valuable insight into its broader applicability. Secondly, the influence of pile-ups of geometrically necessary dislocations (GNDs) and the resulting kinematic hardening were not accounted for in this study. Incorporating these effects within the proposed approach offers the potential to further improve predictions of microscale strain heterogeneities and should be explored in future work. Finally, it is well established that strain heterogeneities can lead to strain localization, which in turn may trigger damage initiation and propagation. Evaluating the potential of this CPFEM implementation to predict the influence of neighboring grains on crack initiation and propagation provides an additional promising possibility for future research.

Appendices

Appendix A - Build up of internal stresses: case of layered composite produced by roll bonding.

A multilayer composite made of alternating layers of austenitic 316L stainless steel and martensitic 410 stainless steel was produced using hot roll-bonding and analysed by Dr. Edouard De Sonis within Prof. Pascal Jacques's research group. This material combination showed high ductility (thanks to layers made of 316L) and high strength (thanks to AISI410). After bonding, the multilaminate was subjected to cold rolling under a large-draught configuration to a total thickness reduction of 60%.

The plastic anisotropy of such roll-bonded composite depends on the mechanical response, and hence the crystallographic textures of its constituents. As outlined in Section 2.1, FCC and BCC metals develop distinct rolling textures. The coexistence of metals of different phase, in which texture induces specific anisotropy, may therefore promote the development of internal stresses during co-deformation, as discussed in Chapter 3. This motivated a further investigation into the possible emergence of internal stresses within the present multilayer.

EBSD analyses (using a step size of $1.79\ \mu\text{m}$) confirmed that each layer developed markedly different textures, consistent with the underlying crystallographic structure (Figure A.1). The 316L austenitic layers exhibited a pronounced brass-type texture, dominated by Brass $\{011\}\langle 211 \rangle$ and Goss $\{011\}\langle 100 \rangle$ components, as typically observed in low stacking-fault-energy alloys subjected to substantial cold reduction (Leffers and Ray, 2009). EBSD observations confirmed a high density of deformation twins. In contrast, the martensitic 410 stainless steel layers displayed a strong α -fibre texture with important rotated cubic $\{001\}\langle 110 \rangle$ component, along with a weaker γ -fiber. Similar texture features have been already reported for AISI 430 martensitic stainless steel after 50% cold rolling (Moura et al., 2022). Corresponding pole figures and ODF sections of the two textures are shown in Figure A.2.

Predictions of internal stress development using CPFEM or mean-field models, as performed in Chapter 3, were not achieved for this multi-laminate.

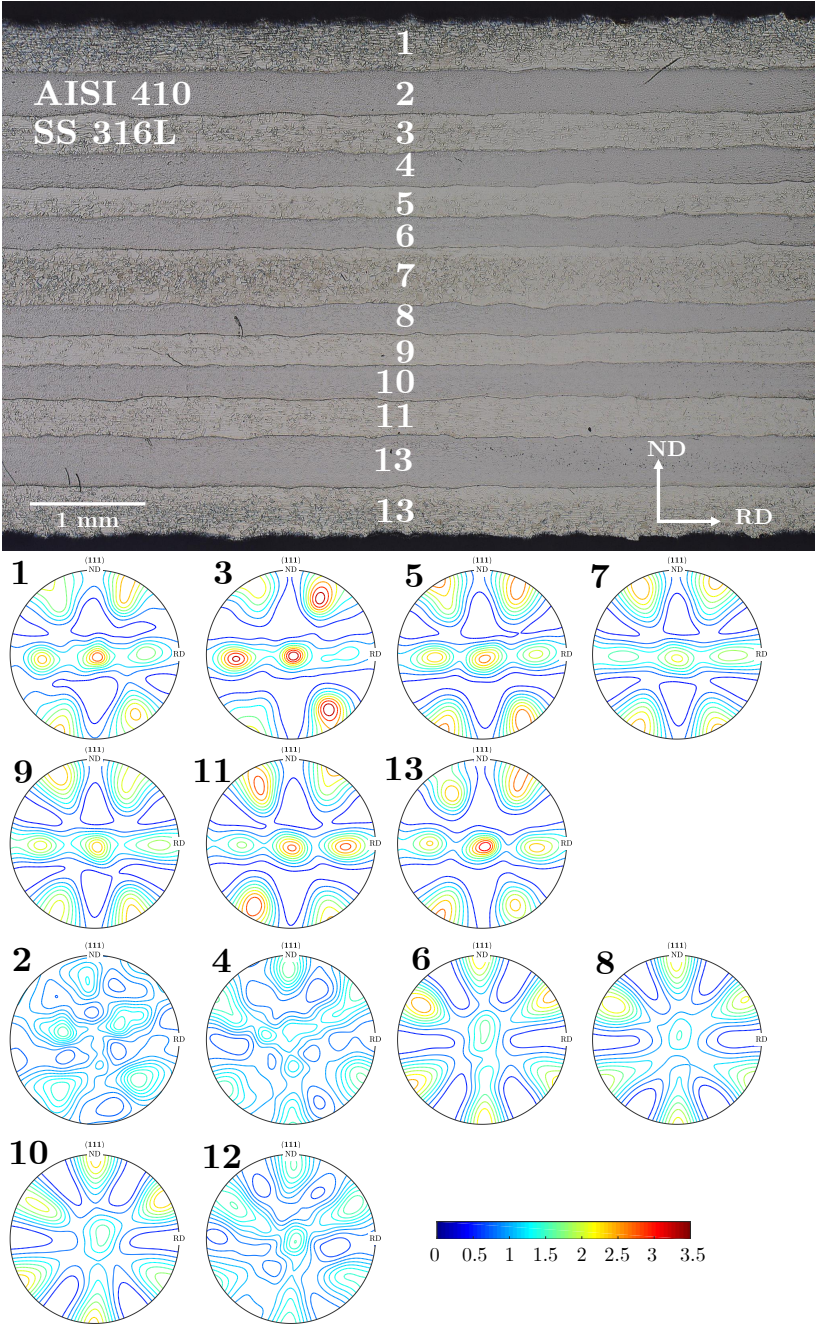


Figure A.1: Characterization of texture and microstructure based on EBSD and optical microscopy. {111} Pole figures (numbered according to the position in the stacking) present the texture developed inside each layer in with the rolling direction (RD) pointing to the right and the normal direction (ND) pointing to the top.

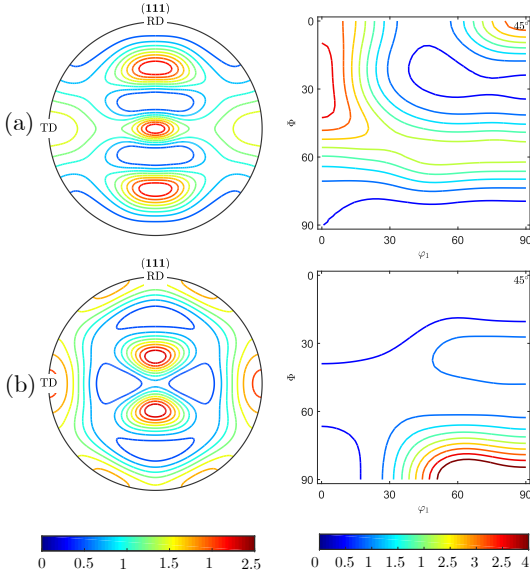


Figure A.2: $\{111\}$ Pole figures in the RD-ND plan and Orientation distribution function (ODF) of (a) martensitic 410 stainless steel (layer 8) and (b) austenitic 316L stainless steel (layer 6).

	$\bar{R}$	ΔR
AISI430 (Vaughan et al., 2022)	0.93	0.45
Pb-Ca-Sn alloy (Abouhilou et al., 2011)	0.43	0.36

Table A.1: Lankford coefficients of metals presenting the same textures than those observed in the studied multilayer.

The crystal-plasticity framework used in this work considers only dislocation glide to realize plastic deformation and does not capture the contributions of deformation twinning or the presence of martensitic phases. Instead, insight into the incompatibility of plastic anisotropy between layers was obtained by examining Lankford coefficients reported in the literature for materials exhibiting similar textures. Cold-rolled Pb-0.08Ca-2Sn, which developed a brass-type texture after 75% reduction (Abouhilou et al., 2011), and cold-rolled AISI 430 (76% thickness reduction), which developed strong α - and γ -fibres (Vaughan et al., 2022), provided representative reference values (Table A.1).

Using the Lankford curve reported in Abouhilou et al. (2011) and assuming $R_0 \simeq R_{90}$ to reconstruct the Lankford curve from Vaughan et al. (2022), approximations of the q -values were derived for each constituent layer (Figure A.3). Both curves exhibited convex shape, yet the martensitic 410 layer consistently showed higher q -values over all loading orientations. This indicates that, upon

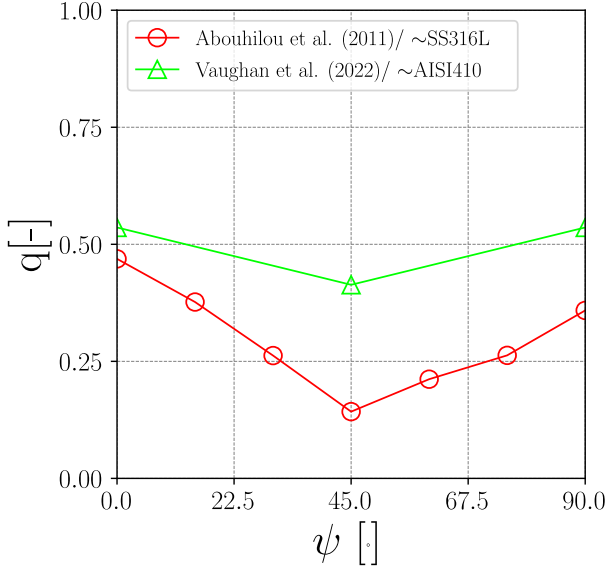


Figure A.3: Estimated q -values corresponding to the textures developed in the two constituent layers, reconstructed from experimental Lankford coefficients reported in Abouhilou et al. (2011); Vaughan et al. (2022).

plastic deformation for any in-plane direction, the AISI 410 layers would experience tensile stresses transverse to the elongation direction, whereas the 316L layers would be in compression in this direction. Furthermore, the difference in normal plastic anisotropy $\bar{R}$ produced by the two textures is significantly larger than that observed for the AA6063 alloy studied in Chapter 3. This suggests that the internal stresses generated by incompatible plastic flow are likely to be more pronounced in the present multilayer system than in the extruded sheet investigated previously.

Overall, the combined texture measurements and estimated anisotropy parameters indicated that substantial internal stresses may develop within the multi-laminate. Further investigations are required to confirm the presence and magnitude of these stresses.

Appendix B - Through-thickness texture gradient in a layered composite produced by roll bonding.

Figure A.2 shows the average texture of each layer of the roll-bonded multilayer described in Appendix A. Comparison of the pole figures corresponding to layers made of the same alloy reveals a progressive rotation of the texture components about the transverse direction (TD) as the distance from the mid-plane increases. This trend is quantified in Figure B.1, which reports the rotation angles $\Delta\varphi_2$ required to restore symmetry about the normal direction (ND) for each layer.

As discussed in Chapter 4, such rotations can be interpreted as the signature of plastic shear strain. The evolution of φ_2 , in Figure B.1, along the thickness suggests an increasing shear deformation toward the sheet surfaces. This distribution aligns with the shear profile typically generated under large rolling draught conditions, which were employed during the cold-rolling passes. It is also interesting to note that the magnitudes of the rotations in layers composed of different alloys are of the same order. It suggests the absence of pronounced shear localization, indicating a better compatibility between AISI 410 and SS316L than that observed for the Fe/Al system in Chapter 4.

The deformation gradient inferred from texture should, however, be confronted with finite-element simulations to confirm this interpretation. This comparison could not be performed using the numerical framework of Chapter 4, as the current crystal-plasticity model accounts only for dislocation glide and does not incorporate deformation twinning or the presence of martensitic phases. Extending the framework to include these contributions would be valuable for validating the proposed shear-strain distribution and to confirm the potential of texture analysis as an indicator of plastic strain gradients in multilayer systems.

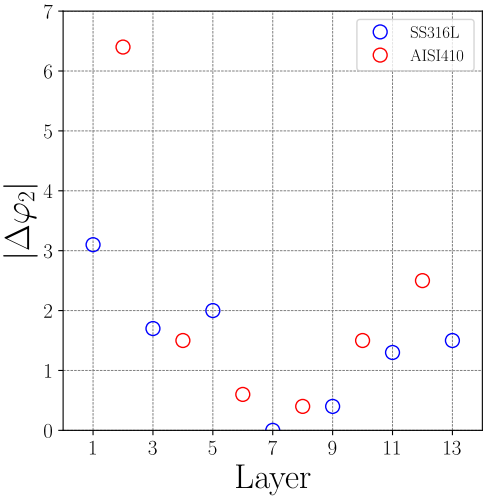


Figure B.1: Rotation angle $|\Delta\phi_2|$ around the TD axis required to obtain symmetrical pole figures about the ND axis in each layer.

Appendix C - Local texture variations in non-flat layers in a multilaminate.

In the Fe–Al 9-layer multilaminate studied in Section 4.5.2, analysis of the local texture within individual layers, rather than the global layer texture, revealed that the crystallographic orientation was non-uniform due to the presence of instabilities. In this Appendix, two Fe layers exhibiting distinct deformed geometries were investigated. The first layer displayed a curved shape (Figure C.1), while the second exhibited a constricted shape (Figure C.2). Each layer was subdivided into 7 sections. For each section, the normals to the top and bottom surfaces (denoted as a and b) were calculated. The inclination angle θ between each normal and the vertical axis (corresponding to the normal direction, ND) was measured. The average inclination for each section was then calculated as $\frac{\theta_a + \theta_b}{2}$. In addition, the pole figure related to each section was computed. The rotation about the transverse direction (TD) axis required to obtain a symmetrical pole figure, denoted $\Delta\phi$, was also determined. The evolution of both $\frac{\theta_a + \theta_b}{2}$ and $\Delta\phi$ along the layer sections for the wavy and nozzle-shaped layers is presented in Figures C.3 and C.4.

For both layer geometries, the two angles exhibited similar values across the sections, with similar magnitudes and signs across the sections. This correlation is due to rigid-body rotations induced by the layer instabilities, which result in a collective rigid rotation of the crystals inducing rotations of the pole figures. Consequently, these rotations are not associated with plastic deformation.

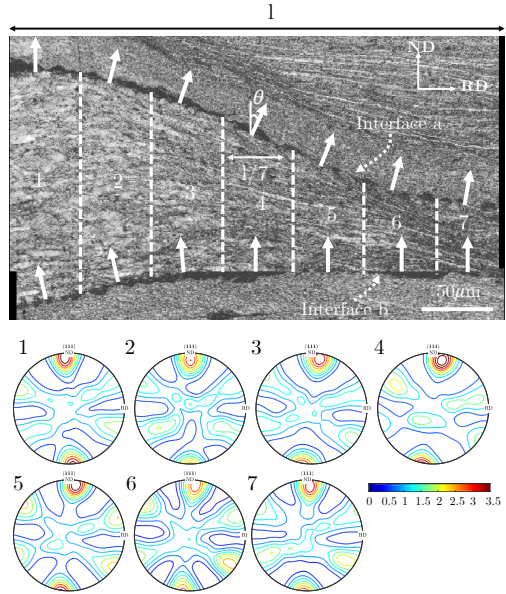


Figure C.1: Iron layer in the 9-layer multilaminate presented in Section 4.5.2 exhibiting a constricted shape. The angle θ represents the inclination of the surface normal with respect to the normal direction (ND). $\{111\}$ pole figures in the RD–ND plane for different sections show a progressive rotation around the TD axis along the layer.

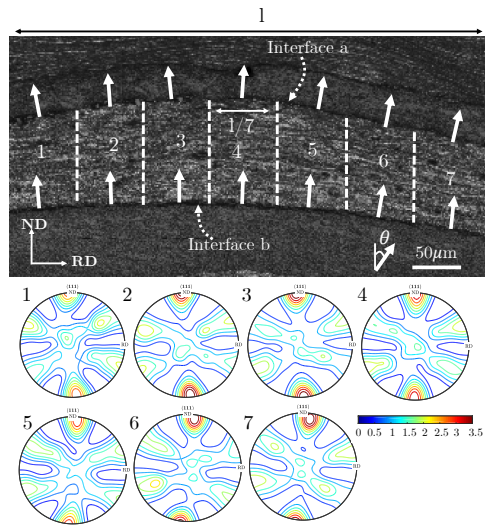


Figure C.2: Iron layer in the 9-layer multilaminate presented in Section 4.5.2 exhibiting a curved shape. The angle θ represents the inclination of the surface normal with respect to the normal direction (ND). $\{111\}$ pole figures in the RD–ND plane for different sections show a progressive rotation around the TD axis along the layer.

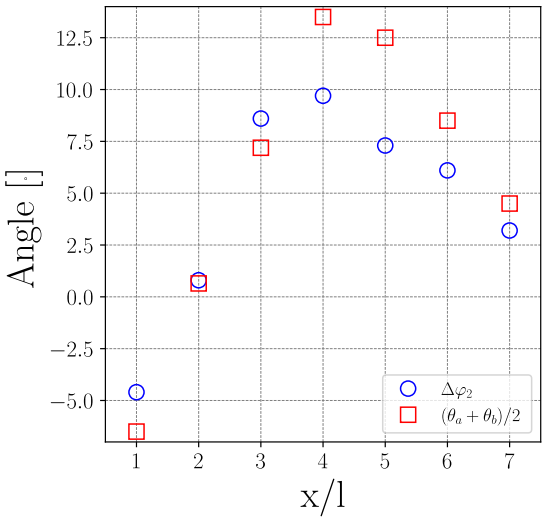


Figure C.3: Average layer inclination ($\frac{\theta_1+\theta_2}{2}$) and rotation of the pole figure ($\Delta\varphi_2$) for the different sections of iron layer having a constricted shape shown in Figure C.1.

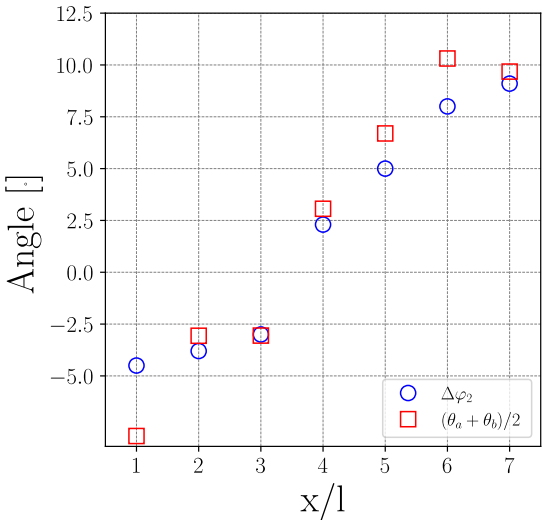


Figure C.4: Average layer inclination ($\frac{\theta_1+\theta_2}{2}$) and rotation of the pole figure ($\Delta\varphi_2$) for the different sections of iron layer having a curved shape shown in Figure C.2.

Appendix D - Quaternion definition and operations.

In crystallography, the orientation of a crystal with respect to a laboratory-fixed frame is commonly described using three Euler angles (φ_1 , Φ , φ_2). These angles define a sequence of three successive rotations required to transform the laboratory frame into the crystal frame: φ_1 corresponds to a rotation about the Z-axis, Φ to a rotation about the X-axis and φ_2 is a rotation around Z-axis. The corresponding global rotation matrix is expressed as:

$$R = \begin{pmatrix} \cos(\varphi_1)\cos(\varphi_2) - \sin(\varphi_1)\sin(\varphi_2)\cos(\Phi) & -\cos(\varphi_1)\sin(\varphi_2) - \sin(\varphi_1)\cos(\varphi_2)\cos(\Phi) & \sin(\varphi_1)\sin(\Phi) \\ \sin(\varphi_1)\cos(\varphi_2) + \cos(\varphi_1)\sin(\varphi_2)\cos(\Phi) & -\sin(\varphi_1)\sin(\varphi_2) + \cos(\varphi_1)\cos(\varphi_2)\cos(\Phi) & -\cos(\varphi_1)\sin(\Phi) \\ \sin(\varphi_2)\sin(\Phi) & \cos(\varphi_2)\sin(\Phi) & \cos(\Phi) \end{pmatrix} \quad (1)$$

An alternative to represent a rotation is to use the quaternions, which offer a compact formulation for performing rotational operations. The quaternion corresponding to the Euler angles are:

$$\begin{cases} q_0 = \cos\left(\frac{\Phi}{2}\right)\cos\left(\frac{\varphi_1+\varphi_2}{2}\right) \\ q_1 = \sin\left(\frac{\Phi}{2}\right)\cos\left(\frac{\varphi_1-\varphi_2}{2}\right) \\ q_2 = \sin\left(\frac{\Phi}{2}\right)\sin\left(\frac{\varphi_1-\varphi_2}{2}\right) \\ q_3 = \cos\left(\frac{\Phi}{2}\right)\sin\left(\frac{\varphi_1+\varphi_2}{2}\right) \end{cases} \quad (2)$$

The rotation matrix can equivalently be expressed in terms of the quaternion components:

$$R = 2 \begin{pmatrix} q_0^2 + q_1^2 - \frac{1}{2} & q_1q_2 - q_0q_3 & q_1q_3 - q_0q_2 \\ q_1q_2 + q_0q_3 & q_0^2 + q_2^2 - \frac{1}{2} & q_2q_3 - q_0q_1 \\ q_1q_3 + q_0q_2 & q_2q_3 - q_0q_1 & q_0^2 + q_3^2 - \frac{1}{2} \end{pmatrix} \quad (3)$$

When combining two successive rotations, represented by rotation matrices R^a and R^b , the resulting rotation matrix is obtained via matrix multiplication:

$$R^{res} = R^b R^a \quad (4)$$

Similarly, the resultant quaternion associated with the combined rotation can be expressed as:

$$\begin{cases} q_0^{res} = q_0^a q_0^b - q_1^a q_1^b - q_2^a q_2^b - q_3^a q_3^b \\ q_1^{res} = q_0^a q_1^b + q_1^a q_0^b + q_2^a q_3^b - q_3^a q_2^b \\ q_2^{res} = q_0^a q_2^b + q_2^a q_0^b + q_3^a q_1^b - q_1^a q_3^b \\ q_3^{res} = q_0^a q_3^b + q_3^a q_0^b + q_1^a q_2^b - q_1^a q_2^b \end{cases} \quad (5)$$

Appendix E - Numerical implementation of Taylor FC, Taylor RC and ALAMEL.

Algorithm 2 Taylor Full-Constraint

Input: $L_{macro}|_{t+\Delta t}$

Output: $R^*|_{t+\Delta t}, \sigma|_{t+\Delta t}$

for crystal **do**

$T|_{t+\Delta t} = T|_t$

$\tau_c|_{t+\Delta t} = \tau_c|_t$

while $\|T^i - T^{i+1}\| > tol$ **do**

▷ N-R scheme

$L_{macro}, \Omega^{i-1}, \dot{\gamma}^{\alpha, i-1} \rightarrow T^i$

▷ Equations 2.57, 2.58

while $\|\tau_c^j - \tau_c^{j+1}\| > tol$ **do**

▷ N-R scheme

$T^i \rightarrow \Delta\gamma^\alpha$

▷ Equations 2.58, 2.59, 2.60

$\Delta\gamma^\alpha \rightarrow \tau_c^{j+1}$

▷ Equations 2.59, 2.60

end while

$\dot{\gamma}^{\alpha, i} \rightarrow L_p^i$

▷ Equation 2.37

$L_{macro}, L_p^i \rightarrow \Omega^{*, i}, R^{*, i}$

▷ Equation 2.62

$L_{macro}, \Omega^{*, i}, \dot{\gamma}^{\alpha, i} \rightarrow T^{i+1}$

▷ equation 2.57

end while

$T|_{t+\Delta t}, R^*|_{t+\Delta t} \rightarrow \sigma|_{t+\Delta t}$

▷ Equation 2.63

end for

Algorithm 3 Taylor Relaxed-Constraint

Input: $L_{macro}|_{t+\Delta t}$
Output: $R^*|_{t+\Delta t}, \sigma|_{t+\Delta t}$
for crystal **do**

$$T|_{t+\Delta t} = T|_t$$

$$\tau_c|_{t+\Delta t} = \tau_c|_t$$

$$\dot{\gamma}_{rlx}|_{t+\Delta t} = \dot{\gamma}_{rlx}|_t$$

while $\|T^i - T^{i+1}\| > tol$ and $|\sigma : (d \otimes n)| > tol$ **do** ▷ N-R scheme

$$L_{macro}, \Omega^{*,i-1}, \dot{\gamma}^{\alpha,i-1} \rightarrow T^i, \dot{\gamma}_{rlx} \quad \text{▷ Eq. 2.58, 2.57, 2.25}$$

$$L_{macro}, \dot{\gamma}_{rlx} \rightarrow L \quad \text{▷ Eq. 2.24}$$

while $\|\tau_c^j - \tau_c^{j+1}\| > tol$ **do** ▷ N-R scheme

$$T^i \rightarrow \Delta \gamma^\alpha \quad \text{▷ Eq.s 2.58, 2.59, 2.60}$$

$$\Delta \gamma^\alpha \rightarrow \tau_c^{j+1} \quad \text{▷ Eq. 2.59, 2.60}$$

end while

$$\dot{\gamma}^{\alpha,i} \rightarrow L_p^i \quad \text{▷ Eq. 2.37}$$

$$L, L_p^i \rightarrow \Omega^{*,i}, R^{*,i} \quad \text{▷ Eq. 2.62}$$

$$L, \Omega^{*,i}, \dot{\gamma}^{\alpha,i} \rightarrow T^{i+1} \quad \text{▷ Eq. 2.57}$$

$$T|_{t+\Delta t}, R^*|_{t+\Delta t} \rightarrow \sigma|_{t+\Delta t} \quad \text{▷ Eq. 2.63}$$

end while
end for

Algorithm 4 ALAMEL

Input: $L_{macro}|_{t+\Delta t}$

Output: $R^*|_{t+\Delta t}, \sigma|_{t+\Delta t}$

for lamel **do**

$$T|_{t+\Delta t, gr1} = T|_{t, gr1}$$

$$T|_{t+\Delta t, gr2} = T|_{t, gr2}$$

$$\tau_c|_{t+\Delta t, gr1} = \tau_c|_{t, gr1}$$

$$\tau_c|_{t+\Delta t, gr2} = \tau_c|_{t, gr2}$$

$$\dot{\gamma}_{rlx}|_{t+\Delta t} = \dot{\gamma}_{rlx}|_t$$

while $\left\| T_{gr1,2}^i - T_{gr1,2}^{i+1} \right\| > tol$ **and** $|(\sigma_{gr1} - \sigma_{gr2}) : (d \otimes n)| > tol$ **do**

2.27 $L_{macro}, \Omega_{gr}^{i-1}, \dot{\gamma}_{gr}^{\alpha, i-1} \rightarrow T_{gr}^i; \dot{\gamma}_{rlx}$ $\triangleright$ N-R scheme: equation 2.58 2.57

$$L_{macro}, \dot{\gamma}_{rlx} \rightarrow L_{gr}$$

for grain **do**

while $\left\| \tau_{c,gr}^j - \tau_{c,gr}^{j+1} \right\| > tol$ **do**

$$T_{gr}^i \rightarrow \Delta \gamma_{gr}^{\alpha} \quad \triangleright \text{N-R scheme: equations 2.58, 2.59, 2.60}$$

$$\Delta \gamma_{gr}^{\alpha} \rightarrow \tau_{c,gr}^{j+1} \quad \triangleright \text{equations 2.59, 2.60}$$

end while

$$\dot{\gamma}_{gr}^{\alpha, i} \rightarrow L_{p,gr}^i \quad \triangleright \text{Equation 2.37}$$

$$L, L_{p,gr}^i \rightarrow \Omega_{gr}^i, R_{gr}^{*,i} \quad \triangleright \text{Equation 2.62}$$

$$L_{gr}, \Omega_{gr}^i, \dot{\gamma}_{gr}^{\alpha, i} \rightarrow T_{gr}^{i+1} \quad \triangleright \text{equation 2.57}$$

end for

$$T_{gr}|_{t+\Delta t}, R_{gr}^*|_{t+\Delta t} \rightarrow \sigma_{gr}|_{t+\Delta t} \quad \triangleright \text{Equation 2.63}$$

end while

end for

Appendix F - Implementation of periodic boundary condition (PBC).

A periodic geometry imposes a well-defined relationship between pairs of nodes situated on opposite outer faces. For any two aligned nodes, labeled A and B, located on faces whose outward normal is oriented along the i -th direction, the difference in their coordinates along that i -th direction is constant and expressed as:

$$x_{i,A} - x_{i,B} = l_i \quad (6)$$

Where $x_{i,A}$ and $x_{i,B}$ represent the coordinates of nodes A and B in the i -th direction, respectively. The parameter l_i corresponds to the translational distance required to superimpose the two opposite faces, ensuring periodicity. This distance remains uniform for all nodes on the same face, as they are equidistant from the opposing face. For the geometry to exhibit perfect periodicity, the coordinates in all the normal directions to direction i must satisfy:

$$x_{j,A} - x_{j,B} = 0, \quad \text{when } j \neq i \quad (7)$$

This inherent periodicity facilitates the implementation of periodic boundary conditions (PBCs), which enforce a kinematic constraint between node pairs. Specifically, PBCs couple the displacements of nodes A and B such that their relative motion reflects the applied deformation gradient as illustrated in Figure F.1.

The relationship between the displacements of node A ($u(A)$) and node B ($u(B)$) in the i -th direction is expressed as:

$$u_i(A) - u_i(B) = \sum_j l_i (F_{ij} - \delta_{ij}) \quad (8)$$

Where δ_{ij} is the Kronecker symbol and F_{ij} is the prescribed deformation gradient. PBCs are applied to all pairs of opposite faces, irrespective of their orientation, ensuring that no free surfaces exist within the periodic structure.

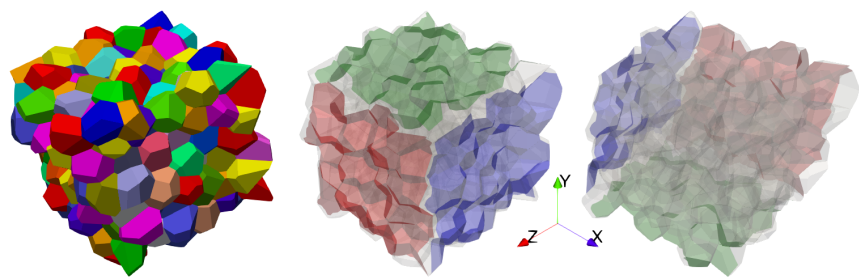


Figure F.1: Periodic Boundary Conditions (PBC) are used to connect opposite faces of a microstructure with a periodic geometry. Faces that share the same color are linked together through PBC.

Appendix G - Equivalent plastic strain rate near crystalline interfaces.

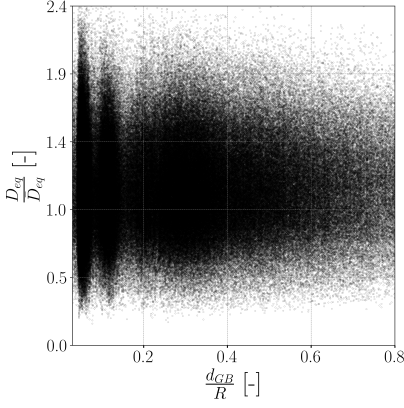


Figure G.1: Local equivalent strain rate at each integration point as a function of the normalized distance to the nearest grain boundary.

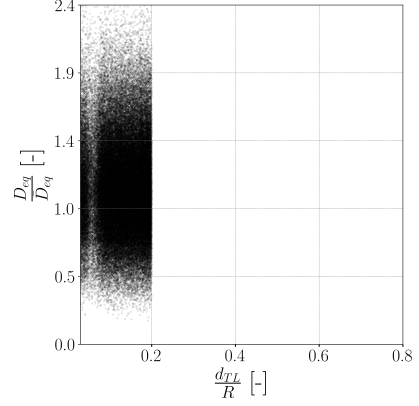


Figure G.2: Local equivalent strain rate at each integration point as a function of the normalized distance to the nearest triple line.

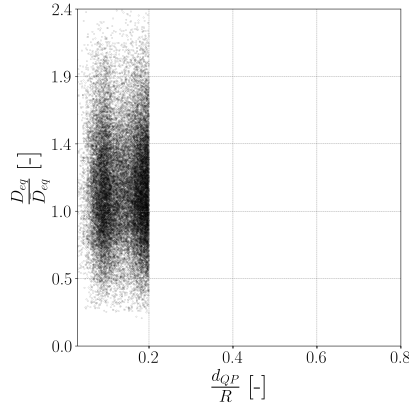


Figure G.3: Local equivalent strain rate at each integration point as a function of the normalized distance to the nearest quadruple point.

Appendix H - Derivation of a scalar metric to characterize strain-rate heterogeneity across a grain boundary.

This section details the development of a scalar metric designed to assess the extent to which the strain-rate heterogeneity across a grain boundary is attributable to shear deformation parallel to that boundary.

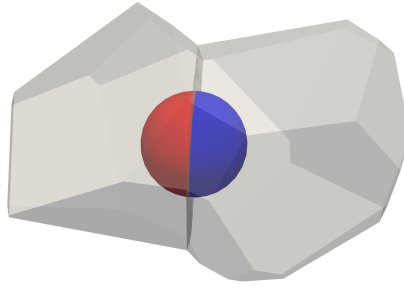


Figure H.1: Illustration of the virtual sphere centred at the barycentre of a grain boundary and partitioned into two half-spheres associated with the adjacent grains.

To characterize the strain-rate state on each side of the boundary, a virtual sphere is constructed around the boundary barycentre and partitioned into two half-spheres corresponding to the adjacent grains (Figure H.1). The strain rate associated with each half-sphere, denoted $\dot{\epsilon}$, is defined as the average strain-rate tensor over all integration points contained within that half-sphere. In the reference coordinate system, this tensor is expressed as:

$$\dot{\epsilon} = \begin{pmatrix} \langle \dot{\epsilon}_{xx} \rangle & \langle \dot{\epsilon}_{xy} \rangle & \langle \dot{\epsilon}_{xz} \rangle \\ \langle \dot{\epsilon}_{yx} \rangle & \langle \dot{\epsilon}_{yy} \rangle & \langle \dot{\epsilon}_{yz} \rangle \\ \langle \dot{\epsilon}_{zx} \rangle & \langle \dot{\epsilon}_{zy} \rangle & \langle \dot{\epsilon}_{zz} \rangle \end{pmatrix}$$

The strain-rate heterogeneity across the boundary is defined as the difference between the tensors characterising the two half-spheres:

$$\delta \dot{\epsilon} = \dot{\epsilon}_{\text{blue}} - \dot{\epsilon}_{\text{red}} = \begin{pmatrix} \Delta \dot{\epsilon}_{xx} & \Delta \dot{\epsilon}_{xy} & \Delta \dot{\epsilon}_{xz} \\ \Delta \dot{\epsilon}_{yx} & \Delta \dot{\epsilon}_{yy} & \Delta \dot{\epsilon}_{yz} \\ \Delta \dot{\epsilon}_{zx} & \Delta \dot{\epsilon}_{zy} & \Delta \dot{\epsilon}_{zz} \end{pmatrix}$$

To interpret the heterogeneity in a boundary-attached reference frame, $\Delta \dot{\epsilon}$ is rotated into a local system (1,2,3) in which axis 3 is normal to the grain boundary. Using the corresponding rotation matrix $\mathbf{R}$, one obtains:

$$\Delta \dot{\epsilon}' = \begin{pmatrix} \Delta \dot{\epsilon}_{11} & \Delta \dot{\epsilon}_{12} & \Delta \dot{\epsilon}_{13} \\ \Delta \dot{\epsilon}_{21} & \Delta \dot{\epsilon}_{22} & \Delta \dot{\epsilon}_{23} \\ \Delta \dot{\epsilon}_{31} & \Delta \dot{\epsilon}_{32} & \Delta \dot{\epsilon}_{33} \end{pmatrix} = \mathbf{R} \begin{pmatrix} \Delta \dot{\epsilon}_{xx} & \Delta \dot{\epsilon}_{xy} & \Delta \dot{\epsilon}_{xz} \\ \Delta \dot{\epsilon}_{yx} & \Delta \dot{\epsilon}_{yy} & \Delta \dot{\epsilon}_{yz} \\ \Delta \dot{\epsilon}_{zx} & \Delta \dot{\epsilon}_{zy} & \Delta \dot{\epsilon}_{zz} \end{pmatrix} \mathbf{R}^T$$

The shear components $\Delta\dot{\epsilon}_{13}$ and $\Delta\dot{\epsilon}_{23}$ correspond to the shear rate parallel to the boundary plane. To rigorously quantify their relative contribution to the overall strain-rate heterogeneity while ensuring geometric invariance with respect to arbitrary rotations of axes 1 and 2 within the boundary plane, a scalar metric λ is defined using the Frobenius norm as:

$$\lambda = \frac{\sqrt{2(\Delta\dot{\epsilon}_{13}^2 + \Delta\dot{\epsilon}_{23}^2)}}{\|\Delta\dot{\epsilon}'\|} = \frac{\sqrt{2(\Delta\dot{\epsilon}_{13}^2 + \Delta\dot{\epsilon}_{23}^2)}}{\sqrt{\Delta\dot{\epsilon}_{11}^2 + \Delta\dot{\epsilon}_{22}^2 + \Delta\dot{\epsilon}_{33}^2 + 2(\Delta\dot{\epsilon}_{12}^2 + \Delta\dot{\epsilon}_{13}^2 + \Delta\dot{\epsilon}_{23}^2)}}$$

Note that λ^2 is naturally bounded between 0 and 1. Consequently, the complementary fraction, $1 - \lambda^2$, accurately encompasses all remaining heterogeneity modes, namely the normal stretching/compression differences across the boundary and the in-plane shear $\Delta\dot{\epsilon}_{12}$.

Appendix I - Distance to the nearest grain boundary in a microstructure generated using Voronoï tessellation.

Voronoï tessellations are widely employed to generate virtual polycrystalline microstructures suitable for CPFEM simulations. A finite set of crystal seeds is first distributed uniformly within a representative volume. Each seed is then assumed to grow at a uniform rate until it encounters neighboring seeds, producing a periodic geometry. The resulting grain morphology corresponds to a convex polyhedral Voronoï cell. The collection of planar interfaces delimiting these cells forms the Voronoï diagram. In the context of CPFEM, these interfaces correspond to the grain boundaries. Several geometric properties of Voronoï diagrams enable the straightforward calculation of distances to the nearest interface

Let the domain $\Omega \subset \mathbb{R}^3$ contain n uniformly distributed seeds, defined as $S = \{p_1, p_2, p_3, \dots, p_n\} \subseteq \mathbb{R}^3$. The Voronoï cell V_i associated with seed p_i is defined as:

$$V_i = \{x \in \mathbb{R}^3 \mid \|x_i - p_i\| < \|x_i - p_j\|, \forall 1 \leq i \leq n, i \neq j\}$$

Therefore, the domain is partitioned into n cells, whose union recovers the entire domain: $\Omega = \bigcup_{1 \leq i \leq n} V_i$.

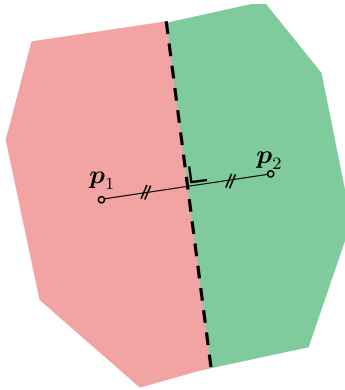


Figure I.1: Segment (solid line) connecting seeds p_1 and p_2 , with its perpendicular bisector (dashed line) coinciding with the interface between the corresponding Voronoï cells.

By construction, the interface separating two neighbouring seeds p_1 and p_2 is the plane perpendicular to the segment joining them and located at its midpoint (the perpendicular bisector), as illustrated in Figure I.1. The outward

unit normal to this interface is:

$$\mathbf{n}_{12} = \frac{\mathbf{p}_2 - \mathbf{p}_1}{\|\mathbf{p}_2 - \mathbf{p}_1\|}$$

This normal vector defines the orientation of the grain boundary plane, but the plane equation also requires an offset coefficient to describe the equation of the plan. Since the interface lies exactly halfway between the two seeds, the plane satisfies:

$$\frac{\|\mathbf{p}_2 - \mathbf{p}_1\|}{2} = n_{12,x}p_{2,x} + n_{12,y}p_{2,y} + n_{12,z}p_{2,z} + d$$

Which allows to calculate the offset coefficient d .

For any point $\mathbf{x} = (x, y, z)$ whose two closest seeds are $\mathbf{p}_1$ and $\mathbf{p}_2$, the signed distance to the grain boundary is thus expressed as:

$$dist = n_{12,x}x + n_{12,y}y + n_{12,z}z + d$$

Appendix J - Validation of the ALAMEL implementation in the UMAT.

The constitutive equations of the ALAMEL model were implemented in the UMAT subroutine for CPFEM simulations to account for a lamella, capturing grain interactions, at each integration point rather than a single crystal. Consequently, the stress tensor at each integration point now corresponds to the stress within a lamella. A validation study was conducted to verify the correct implementation and to assess the accuracy of the model predictions.

To validate the implementation, the compression deformation of a bicrystal was investigated. Two types of simulations were performed (Figure J.1):

1-brick simulation: A single hexahedral element (C3D8) represented both grains. The same crystallographic orientations and the same normal direction to the grain boundary were assigned at each integration point. Periodic boundary conditions were applied, while prescribed boundary conditions were:

$$\langle F \rangle_{\Omega} = \begin{pmatrix} ? & 0 & 0 \\ 0 & -0.2 & 0 \\ 0 & 0 & ? \end{pmatrix} \quad \langle \sigma \rangle_{\Omega} = \begin{pmatrix} 0 & ? & ? \\ ? & ? & ? \\ ? & ? & 0 \end{pmatrix}$$

2-brick simulation: A mesh consisting of two stacked C3D8 elements was used. Each element represents a single grain with a unique crystallographic orientation. The interface normal between the elements is aligned with the y -direction of the global coordinate system. To maintain mechanical equivalence with the 1-brick case, a rigid body rotation $\Delta\varphi_2$ was applied to the initial Euler angles of both grains. This rotation aligns the grain boundary orientation used in the 1-brick case with the y -axis of the 2-brick case. Consequently, the boundary conditions were also transformed to remain consistent with the rotated reference frame.

The validation focused on two specific grain boundary inclinations, defined by the angle between the x -direction and the grain boundary in the 1-brick simulation frame (Fig. J.2):

- Case 1: An inclination of $+45^\circ$.
- Case 2: An inclination of -63° .

The fidelity of the implementation was assessed by comparing the strain rate tensors $\dot{\epsilon}_{A,B}$ of each grain and the final crystallographic orientations (texture evolution) predicted by the 2-brick model against the results obtained from the 1-brick simulation.

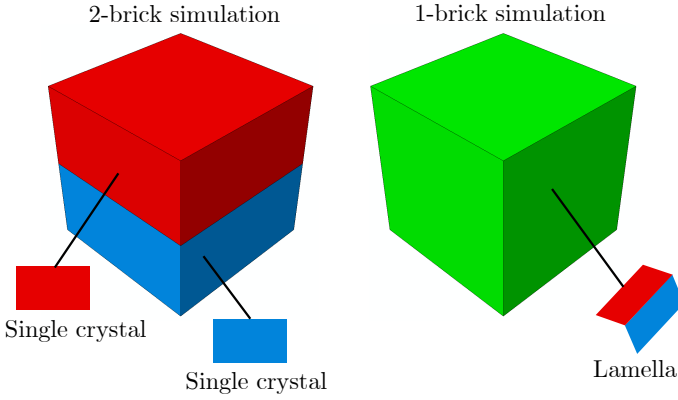


Figure J.1: Illustration of the two types of simulation used for the validation. In the 1-brick simulation, each integration point behaves as a lamella, whereas in the 2-brick simulation each integration point corresponds to a single crystal associated with the element in which it is located.

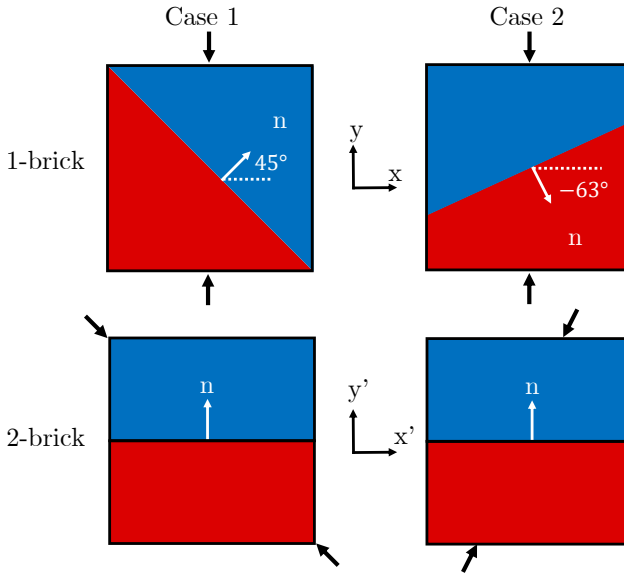


Figure J.2: Illustration of the two cases investigated for validation. The 1-brick simulation corresponds to a uniaxial compression test, whereas in the 2-brick simulation the loading direction and the Euler angles were adjusted to ensure a consistent comparison with the 1-brick configuration. The illustrations are shown in the coordinate systems used in their respective simulations.

Case 1: 45° Grain Boundary Inclination

The initial crystallographic orientations assigned to the two grains are listed in Table J.1.

t_0	φ_1	Φ	φ_2
Grain A	20.5°	19.5°	199.9°
Grain B	0.8	39.3°	66.39

Table J.1: Initial crystallographic orientations used in case 1.

The 2-brick simulation predicted the following strain rate tensors in the simulation frame:

$$\dot{\epsilon}_A = \begin{pmatrix} -0.013852 & 0.1263 & -0.0063835 \\ 0.1263 & -0.070915 & 0.036653 \\ -0.0063835 & 0.036653 & 0.084483 \end{pmatrix}$$

$$\dot{\epsilon}_B = \begin{pmatrix} -0.071193 & 0.286 & 0.0063775 \\ 0.286 & -0.014184 & -0.0366185 \\ 0.0063775 & -0.0366185 & 0.084483 \end{pmatrix}$$

After transformation to the frame used in the 1-brick simulation, these tensors become:

$$\dot{\epsilon}_A = \begin{pmatrix} 0.0839165 & -0.0285315 & 0.02140377 \\ -0.0285315 & -0.1686835 & 0.0304314 \\ 0.02140377 & 0.0304314 & 0.084483 \end{pmatrix}$$

$$\dot{\epsilon}_B = \begin{pmatrix} 0.2433115 & 0.0285045 & -0.02138362 \\ 0.0285045 & -0.3286885 & -0.03040276 \\ -0.02138362 & -0.03040276 & 0.084483 \end{pmatrix}$$

The corresponding macroscopic strain rate tensor, obtained as the average of the two grains, is:

$$\langle \dot{\epsilon} \rangle_{\Omega} = \frac{\dot{\epsilon}_A + \dot{\epsilon}_B}{2} = \begin{pmatrix} 0.163614 & -0.0000135 & 0.000010075 \\ -0.0000135 & -0.248686 & 0.00001432 \\ 0.000010075 & 0.00001432 & 0.084483 \end{pmatrix}$$

The 1-brick simulation predicted a macroscopic strain rate tensor of:

$$\langle \dot{\epsilon} \rangle_{\Omega} = \begin{pmatrix} 0.1633 & 0 & 0 \\ 0 & -0.2488 & 0 \\ 0 & 0 & 0.084844 \end{pmatrix}$$

Using the relaxation shear rates along the grain boundary predicted by ALAMEL ($\dot{\gamma}_1 = -0.1758$ and $\dot{\gamma}_2 = -0.065099$), the strain rate tensor for each grain can be reconstructed as:

$$\dot{\epsilon}_{A,B} = \langle \dot{\epsilon} \rangle_{\Omega} \pm \widehat{\mathbf{R}} \begin{pmatrix} 0 & 0 & \frac{\dot{\gamma}_1}{2} \\ 0 & 0 & \frac{\dot{\gamma}_2}{2} \\ \frac{\dot{\gamma}_1}{2} & \frac{\dot{\gamma}_2}{2} & 0 \end{pmatrix} \widehat{\mathbf{R}}^T$$

Where $\widehat{\mathbf{R}}$ transforms tensors from the crystal frame to the reference frame. This gives:

$$\dot{\epsilon}_A = \begin{pmatrix} 0.08044396 & -0.02934171 & 0.01878763 \\ -0.02934171 & -0.16595014 & 0.0265774 \\ 0.01878763 & 0.0265774 & 0.0848414 \end{pmatrix}$$

$$\dot{\epsilon}_B = \begin{pmatrix} 0.24615604 & 0.02934171 & -0.01878763 \\ 0.02934171 & -0.33164986 & -0.0265774 \\ -0.01878763 & -0.0265774 & 0.0848466 \end{pmatrix}$$

Both the macroscopic and individual grain strain rates predicted by the two simulations are in close agreement. The final crystallographic orientations, summarized in Table J.2, also show excellent agreement.

t_{final}	φ_1	Φ	φ_2
Grain A - 2-brick	39.316	15.624	187.754
Grain A - 1-brick	39.787°	15.550°	187.143°
Grain B - 2-brick	8.614	39.079	68.920 °
Grain B - 1-brick	8.672°	39.140°	68.911°

Table J.2: Final crystallographic orientations of both grains after loading, as predicted by the 1-brick and 2-brick simulations for Case 1.

Configuration 2: -63° GB inclined

The initial crystallographic orientations assigned to the two grains are listed in Table J.3.

t_0	φ_1	Φ	φ_1
Grain A	312.5°	35°	45°
Grain B	107.5°	82.5°	57.5°

Table J.3: Crystallographic orientations used in case 2.

The 2-brick simulation predicted the following strain rate tensors in the simulation frame:

$$\dot{\epsilon}_A = \begin{pmatrix} 0.094786 & -0.16615 & -0.0102115 \\ -0.16615 & -0.1624 & -0.07135 \\ -0.0103175 & -0.07135 & 0.067046 \end{pmatrix}$$

$$\dot{\epsilon}_B = \begin{pmatrix} 0.090276 & -0.1816 & 0.0102 \\ -0.1816 & -0.1578 & 0.0713 \\ 0.0102 & 0.0713 & 0.067046 \end{pmatrix}$$

Transforming these tensors to the frame used in the 1-brick simulation gives:

$$\dot{\epsilon}_A = \begin{pmatrix} 0.17619624 & 0.0063734 & 0.02329371 \\ 0.0063734 & -0.24381024 & -0.06820924 \\ 0.02329371 & -0.06820924 & 0.067046 \end{pmatrix}$$

$$\dot{\epsilon}_B = \begin{pmatrix} 0.18606319 & -0.00639295 & -0.02328126 \\ -0.00639295 & -0.25358719 & 0.06815947 \\ -0.02328126 & 0.06815947 & 0.067046 \end{pmatrix}$$

$$\langle \dot{\epsilon} \rangle_{\Omega} = \frac{\dot{\epsilon}_A + \dot{\epsilon}_B}{2} = \begin{pmatrix} 0.181129718 & -0.000009774588 & 0.00000622647 \\ -0.00000977458758 & -0.248698718 & -0.0000248856 \\ 0.00000622647498 & -0.0000248856 & 0.067046 \end{pmatrix}$$

For comparison, the 1-brick simulation predicted a macroscopic strain rate tensor of:

$$\begin{pmatrix} 0.1822 & 0 & 0 \\ 0 & -0.249 & 0 \\ 0 & 0 & 0.06622 \end{pmatrix}$$

Using the relaxation shear rates along the grain boundary predicted by ALAMEL ($\dot{\gamma}_1 = 0.0185395$ and $\dot{\gamma}_2 = 0.1387$), the strain rate tensor for each grain can be reconstructed:

$$\dot{\epsilon}_A = \begin{pmatrix} 0.17650564 & 0.00731782 & 0.02252528 \\ 0.00731782 & -0.24331946 & -0.06560609 \\ 0.02252528 & -0.06560609 & 0.06620468 \end{pmatrix}$$

$$\dot{\epsilon}_B = \begin{pmatrix} 0.18789436 & -0.00731782 & -0.02252528 \\ -0.00731782 & -0.25468054 & 0.06560609 \\ -0.02252528 & 0.06560609 & 0.06623532 \end{pmatrix}$$

Both the macroscopic and individual grain strain rates predicted by the two simulations are in close agreement. The final crystallographic orientations, summarized in Table J.4, also show excellent agreement.

For both studied case, the 1-brick simulation gave results very similar to those of the 2-brick simulation, which was used as a benchmark. This confirms that the ALAMEL hypotheses were correctly implemented.

t_{final}	φ_1	Φ	φ_2
Grain A - CPFEM	319.511°	36.259°	46.193°
Grain A - ALAMEL	319.51°	36.253°	46.176°
Grain B - CPFEM	101.822°	84.078°	61.63°
Grain B - ALAMEL	101.801°	84.089°	61.631°

Table J.4: Final crystallographic orientations of both grains after loading, as predicted by the 1-brick and 2-brick simulations for Case 2.

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