OBSERVATION AND MODELLING
OF GRAIN INTERACTIONS
AND GRAIN SUBDIVISION
IN ROLLED CUBIC POLYCRYSTALS

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in de toegepaste wetenschappen
door
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Foreword

Just like the plastic deformation of a grain embedded in a polycrystalline aggregate is significantly influenced by interactions with the surrounding grains, I could carry out this work thanks to the many fruitful and motivating contacts that I had with researchers and friends around me.

In first instance, I wish to express my gratitude to Professors P. Van Houtte and E. Aernoudt who have supervised this work both with valuable expertise and with a kind, careful attention in my progresses. Repeatedly, I was impressed by their competency as researchers and by their will to know ever more about texture and micromechanics. I realise that the task, which they assigned to me initially, was one with many promises and that it strongly relied on the modern experimental equipment made available in MTM (OIM, XRD, …). By inviting outstanding researchers to visit MTM, by permitting interactions with the Belgian industry and by sending me to diverse conferences and workshops abroad, my supervisors gave me opportunities to discuss even my early naïve results with the most renown personalities in our field. I appreciate the thrust shown by my supervisors in letting me decide how to orient my research during its progress.

Besides my supervisors, I am grateful to Professors B. Verlinden and B. Blanpain who, after a thorough preliminary examination of the text, suggested useful corrections. I am also thankful to the other members of the jury: Professors J. Berlamont, J. Driver, and L. Froyen for the time spent in evaluating this thesis.

In the course of my first year at MTM, I discovered crystallographic textures by elaborating a new parameter model for the characterisation of steel plate textures. Many thanks to Bert Van Bael, Leo Kestens and Dirk Vanderschueren for their support and their helpful comments all along this preliminary investigation and after.

It is still a mystery to me how the thesis that I wrote could contain more experimental results than mathematical equations. Certainly, this was achieved thanks to the instructive and kind assistance of my colleagues Peter Ratchev and Indra Samajdar experts in the microstructural observation of aluminium plates. Of equal importance were the skills and the know-how of our technical staff. I address my gratitude to Rudy De Vos and Luc Boon for the maintenance of the OIM equipment and to Louis Depré for the XRD measurements.
My one-month stay at the Risø National Laboratory (Denmark) was also extremely beneficial to the experimental work reported in this thesis. Among the many researchers who have helped me and advised me there, I wish to thank specifically Oleg Mishin and Dorte Juul Jensen. Their experienced remarks and their friendly support were precious throughout our collaboration, leading to the results presented in Chapter 5.

The finite element simulations that I carried out rely on the software developed by Surya Kalidindi. Through his intelligent advice and his enthusiasm in our discussions during and after his stay at MTM, he was a driving force of my research.

I acknowledge my grant as Aspirant of the Fonds voor Wetenschappelijk Onderzoek (FWO) – Vlaanderen. Financial support for this work was also obtained through the FOM 99.1098 project (The Netherlands).

Thank you Eric, Saiyi-li, Laurent, Wojtec, Gijs, Bart, Annelies, Etienne, Marc, Béa, Fred, Catherine, Gert, Sacha, Shen, Brad,… for the Alma lunches, the birthday cakes, the coffee breaks, etc. Our discussions were, let’s admit it, not always scientific but they contributed just as much to my pleasure to come to work everyday.

Enfin, je remercie du fond du cœur ma famille qui, par son soutien permanent, ses conseils judicieux et ses nombreuses attentions, m’a permis de réaliser cette recherche dans des conditions idéales. Merci plus encore à Caro pour sa présence, sa tendresse et son courage à travers 9 mois de grossesse qui m’ont vu fort préoccupé par la rédaction de ma thèse.
Abstract

OBSERVATION AND MODELLING OF GRAIN INTERACTION AND GRAIN SUBDIVISION IN ROLLED CUBIC METALS

In this work, some new hypotheses are tested on how to distribute stresses and strain over the crystallite aggregate constituting a cold rolled metal plate. Four polycrystal plasticity models are applied: the traditional “full constraints” and “relaxed constraints” Taylor models, the recently developed LAMEL model and a grain-scale finite element (FE) model. We demonstrate that, by permitting the interaction of individual grains with a specific neighbourhood, the LAMEL and the FE models yield improved predictions of texture evolution in cold rolled steel and aluminium plates. Then, we check whether neighbour interactions are a predominant driving force for the subdivision of individual grains in a polycrystal. The microstructure of an aluminium sheet (AA1050) cold rolled 40% is studied using orientation imaging microscopy (OIM) and a novel computational method is proposed for a systematic analysis of grain subdivision from the local orientation data. Applying this to 352 grains in 16 orientation maps, a correlation is found between the mean orientation of a grain and the type and level of subdivision. A series of computational experiments are then designed so as to verify whether the LAMEL and/or the FE model predict the experimentally observed orientation effect on subdivision.
Nederlandse samenvatting

OBSERVATIE EN MODELLERING VAN KORRELINTERACTIE EN KORRELSPLITTING IN GEWALSTE KUBISCHE METALEN

In dit werk worden nieuwe hypothese getest i.v.m. de verdeling van spanningen en vervormingen in een polykristallijn metaalplaat gedurende het koudwalsen. Vier theorieën over polykristallijn plasticiteit worden toegepast: de traditionele “full constraints-” en “relaxed constraints-” Taylor modellen, het recent ontwikkelde LAMEL model en een eindige elementen (E-E) model op de korrelschaal. Eerst tonen wij aan dat het LAMEL model en het E-E model, die beide rekening houden met de interactie tussen naburige korrels, de textuurverfouling in koudgewalste aluminium- en staalplaten beter voorspellen. Daarna gaan wij na of de interactie tussen naburige korrels een belangrijke drijvende kracht is voor de splitsing van deze korrels. De microstructuur van een 40%-gewalste aluminiumplaat (AA1050) wordt bestudeerd m.b.v. “orientation imaging microscopy” (OIM) en een nieuwe computermethode wordt voorgesteld voor de systematische analyse van korrelsplitsing vanuit de lokale oriëntatiedata. Door dit toe te passen op 352 korrels in 16 OIM-opnamen, wordt een correlatie gevonden tussen, enerzijds, de gemiddelde kristaloriëntatie en, anderzijds, het type en de mate van splitsing. Een reeks computerexperimenten wordt ontworpen om na te gaan of het LAMEL model en/of het E-E model het experimenteel waargenomen effect van oriëntatie op splitsing kunnen voorspellen.
Symbols and abbreviations

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( b_i)</td>
<td>slip direction of the ( s^{th} ) slip system.</td>
</tr>
<tr>
<td>( C_{j}^{\mu\nu} )</td>
<td>coefficients of the series expansion describing the ODF</td>
</tr>
<tr>
<td>( d_{ij} )</td>
<td>local plastic strain rate</td>
</tr>
<tr>
<td>( d_{eq} )</td>
<td>local equivalent plastic strain rate</td>
</tr>
<tr>
<td>( D_g )</td>
<td>Macroscopically prescribed plastic strain rate</td>
</tr>
<tr>
<td>( f(g) )</td>
<td>orientation distribution function</td>
</tr>
<tr>
<td>( F_{ij} )</td>
<td>deformation tensor</td>
</tr>
<tr>
<td>( g )</td>
<td>shorthand for the three Euler angles that describe a crystal orientation</td>
</tr>
<tr>
<td>( {h k l} )</td>
<td>Miller indices of the slip plane (for slip systems) or of the crystal plane parallel to the rolling plane (for texture components)</td>
</tr>
<tr>
<td>( l_{ij} )</td>
<td>local velocity gradient</td>
</tr>
<tr>
<td>( l_{13} )</td>
<td>local velocity gradient component describing a RD-ND simple shear</td>
</tr>
<tr>
<td>( l_{23} )</td>
<td>local velocity gradient component describing a TD-ND simple shear</td>
</tr>
<tr>
<td>( l_{12} )</td>
<td>local velocity gradient component describing a RD-TD simple shear</td>
</tr>
<tr>
<td>( L_{ij} )</td>
<td>macroscopic velocity gradient</td>
</tr>
<tr>
<td>LMAX</td>
<td>maximum order of the series expansion describing the ODF</td>
</tr>
<tr>
<td>( m )</td>
<td>strain rate sensitivity factor</td>
</tr>
<tr>
<td>( M )</td>
<td>Taylor factor</td>
</tr>
<tr>
<td>( M_{ij} )</td>
<td>geometrical factor equal to ( b_i n_j^s )</td>
</tr>
<tr>
<td>( n )</td>
<td>number of potential slip systems (12 in fcc and 24 in bcc)</td>
</tr>
<tr>
<td>( n_j^s )</td>
<td>normal to the slip plane of the ( s^{th} ) slip system</td>
</tr>
<tr>
<td>( P(\sigma_{ij}) )</td>
<td>viscoplastic equipotential surface</td>
</tr>
<tr>
<td>( r)-value</td>
<td>ratio of the transverse and normal strain rates during a traction test on a plate</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>-------------</td>
<td>------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>$&lt;u\ v\ w&gt;$</td>
<td>Miller indices of the slip direction (for slip systems) or of the crystal</td>
</tr>
<tr>
<td></td>
<td>direction parallel to the rolling direction (for texture components)</td>
</tr>
<tr>
<td>$\dot{W}$</td>
<td>plastic work rate</td>
</tr>
<tr>
<td>$\gamma_s$</td>
<td>dislocation slip rate along the $s^{th}$ slip system</td>
</tr>
<tr>
<td>$\gamma_i^L$, $\gamma_j^L$</td>
<td>pseudo-slips describing the shear relaxation in the LAMEL model</td>
</tr>
<tr>
<td>$\Theta_{CB}$</td>
<td>same definition as $\Theta_{rel}$ but accounting only for the misorientations</td>
</tr>
<tr>
<td></td>
<td>larger than 2°</td>
</tr>
<tr>
<td>$\theta_M$</td>
<td>misorientation between one point in the orientation map and the mean</td>
</tr>
<tr>
<td></td>
<td>orientation of the corresponding grain</td>
</tr>
<tr>
<td>$\Theta_M$</td>
<td>average $\theta_M$ value over a grain mapped by OIM</td>
</tr>
<tr>
<td>$\Theta_M^C$</td>
<td>$\Theta_M$ after correction for the grain area effect</td>
</tr>
<tr>
<td>$\theta_{rel}$</td>
<td>misorientation between two adjacent points in the orientation map</td>
</tr>
<tr>
<td>$\Theta_{rel}$</td>
<td>average $\theta_{rel}$ value over a grain mapped by OIM</td>
</tr>
<tr>
<td>$\varphi_1,\Phi,\varphi_2$</td>
<td>Euler angles (angles of three consecutive rotations bringing the external</td>
</tr>
<tr>
<td></td>
<td>reference frame (RD,TD,ND) onto the crystal lattice)</td>
</tr>
<tr>
<td>$\sigma_{ij}$</td>
<td>deviatoric stress</td>
</tr>
<tr>
<td>$\sigma_{eq}$</td>
<td>equivalent stress</td>
</tr>
<tr>
<td>$\tau_s$</td>
<td>resolved shear stress on the $s^{th}$ slip system</td>
</tr>
<tr>
<td>$\tau_s^c$</td>
<td>critical resolved shear stress on the $s^{th}$ slip system</td>
</tr>
<tr>
<td>$\omega_{ij}$</td>
<td>skew-symmetric part of the local velocity gradient</td>
</tr>
<tr>
<td>$\Omega_{ij}^L$</td>
<td>rate of lattice spin</td>
</tr>
<tr>
<td>bcc</td>
<td>body-centred cubic</td>
</tr>
<tr>
<td>brass</td>
<td>${110}&lt;112&gt;$ texture component</td>
</tr>
<tr>
<td>copper</td>
<td>${112}&lt;111&gt;$ texture component</td>
</tr>
<tr>
<td>cube</td>
<td>${001}&lt;100&gt;$ texture component</td>
</tr>
<tr>
<td>CB</td>
<td>cell block</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>------------</td>
</tr>
<tr>
<td>CI</td>
<td>confidence index</td>
</tr>
<tr>
<td>C.R.</td>
<td>cold rolled</td>
</tr>
<tr>
<td>CSL</td>
<td>coincidence site lattice</td>
</tr>
<tr>
<td>EBSD</td>
<td>electron back-scattering diffraction</td>
</tr>
<tr>
<td>fcc</td>
<td>face-centred cubic</td>
</tr>
<tr>
<td>FC</td>
<td>full constraints</td>
</tr>
<tr>
<td>FE</td>
<td>finite element</td>
</tr>
<tr>
<td>FEG</td>
<td>field emission gun</td>
</tr>
<tr>
<td>hcp</td>
<td>hexagonal close-packed</td>
</tr>
<tr>
<td>IF</td>
<td>interstitial free</td>
</tr>
<tr>
<td>IQ</td>
<td>image quality</td>
</tr>
<tr>
<td>LEDS</td>
<td>low energy dislocation structure</td>
</tr>
<tr>
<td>MB</td>
<td>microband</td>
</tr>
<tr>
<td>ND</td>
<td>normal direction to the rolling plane</td>
</tr>
<tr>
<td>N-site</td>
<td>refers to a plasticity model that considers the interaction of $N$ neighbouring grains</td>
</tr>
<tr>
<td>ODF</td>
<td>orientation distribution function</td>
</tr>
<tr>
<td>OIM</td>
<td>orientation imaging microscopy</td>
</tr>
<tr>
<td>PSC</td>
<td>plane strain compression</td>
</tr>
<tr>
<td>RC</td>
<td>relaxed constraints</td>
</tr>
<tr>
<td>RD</td>
<td>rolling direction</td>
</tr>
<tr>
<td>RDC</td>
<td>${025}&lt;100&gt;$ cube component rotated $22^\circ$ around RD</td>
</tr>
<tr>
<td>S</td>
<td>${123}&lt;634&gt;$ texture component</td>
</tr>
<tr>
<td>SEM</td>
<td>scanning electron microscope/microscopy</td>
</tr>
<tr>
<td>SFE</td>
<td>stacking fault energy</td>
</tr>
<tr>
<td>TD</td>
<td>transverse direction in a rolled plate</td>
</tr>
<tr>
<td>TDC</td>
<td>${205}&lt;502&gt;$ cube component rotated $22^\circ$ around TD</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>------------</td>
</tr>
<tr>
<td>TEM</td>
<td>transmission electron microscope/microscopy</td>
</tr>
<tr>
<td>ULC</td>
<td>ultra low carbon</td>
</tr>
<tr>
<td>XRD</td>
<td>X-ray diffraction</td>
</tr>
<tr>
<td>α-fibre</td>
<td>crystallographic fibre containing all crystal orientations with a $&lt;110&gt;$ direction parallel to RD (in steel)</td>
</tr>
<tr>
<td>β-fibre</td>
<td>crystallographic fibre containing the stable texture components ($brass, S, copper$) during rolling of aluminium</td>
</tr>
<tr>
<td>γ-fibre</td>
<td>crystallographic fibre containing all crystal orientations with a ${111}$ direction parallel to ND (in steel)</td>
</tr>
</tbody>
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4 Texture predictions in aluminium

5 Improvement of the LAMEL model

6 Discussion
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INTRODUCTION

Improving our ability to simulate the micromechanics of polycrystalline materials is a challenge for industrial and academic researchers. If there is one point on which the environmentalist and the economist agree, it is to urge the engineer to reduce the consumption of energy and produce fewer wastes. For optimum performance, durability and safety, it is further required that the designed components be both lighter and mechanically stronger. The thorough understanding of polycrystalline plasticity and its application to the computerised optimisation of forming processes is certainly one of the keys to producing metal components that fulfil these requirements. This, by its own, will allow the fabrication of lighter components with more complex shapes, while taking full advantage of the hardening and the anisotropy that are inherent to the material.

The metal components considered in this thesis are cold rolled steel and aluminium sheets that are used for example in the production of beverage cans and car bodies. These sheets are interesting from an industrial as well as an academic viewpoint. On the one hand, it is recognised that deep drawing simulations yield realistic results only if the mechanical anisotropy of the rolled sheets is accounted for. On the other hand, although the crystallographic texture created during rolling has been clearly identified as the principal cause of this anisotropy, modelling the effect of texture on the mechanical properties of the plate is still not totally successful.

Experience has shown that a correct prediction of the mechanical anisotropy in metal sheets necessitates that the polycrystalline character of the metal is taken into account. This can be carried out by considering that single crystal plasticity is valid within each grain, and by making assumptions about how macroscopic constraints apply to individual grains in the polycrystal. For many years, this “macro to micro” transition relied on the oversimplifying assumption due to Taylor (1939) and according to which all grains undergo the exact same
plastic deformation as that observed macroscopically. However, this assumption is unrealistic because it does not achieve stress equilibrium along grain boundaries. In the real material, grains interact with one another and this gives rise to local strain heterogeneities that partly explain the discrepancies between Taylor predictions and experimental results.

In this work, an attempt is made to replace the classical Taylor theory by a model that accounts for interactions of individual grains with their specific surrounding. Two such models have been selected for comparison with the Taylor theory. One is the LAMEL model (Van Houtte et al, 1999), which assumes that grains are lamellas interacting with a single neighbour at a time. The other is a grain-scale finite element (FE) model that solves the plasticity equations simultaneously for the whole polycrystalline aggregate, ensuring strain compatibility and stress equilibrium everywhere. In fact, the FE model cannot replace the Taylor model in macroscopic simulations because this would require excessive computational power. It is used here to generate a reference material law, orienting further developments of the computationally much faster LAMEL model.

The different plasticity models are first applied to the prediction of rolling textures in steel and in aluminium. Such predictions present obvious industrial interest: a reliable model would permit foreseeing how some changes in the rolling process conditions may affect the final texture. It might even indicate how some textures, which are known to be more suitable for the future application of the plate, can be generated. More fundamentally, the LAMEL model and the FE model should improve rolling texture predictions only if they simulate polycrystalline micromechanics significantly better than the classical Taylor theory. As the principles governing the distribution of stresses and strain among and within the constituting crystallites should also apply under more complex macroscopic strain paths, e.g. deep drawing, it is hoped that using a grain interaction model would also be beneficial in those cases.

However, recording the macroscopic texture evolution can provide only indirect information about the validity of a model at the microscopic scale. More reliable information can be obtained from the “microtexture”, i.e. the formation of intra-granular orientation gradients and the fragmentation of the grain into misoriented volumes. This constitutes the most direct observation of the effect of neighbouring grains on the dislocation slip activity within a grain. In this work, a powerful technique called orientation imaging microscopy
(OIM) is used to investigate grain subdivision in cold rolled aluminium. A computational procedure is proposed for a systematic characterisation of intragranular heterogeneities from the local orientation data.

Then, a series of computational experiments are designed in order to check whether the LAMEL model and/or the FE model can reproduce the OIM findings. The focus is, here, set on the experimentally observed correlation between the mean orientation of a grain and the orientation range developing within the grain due to interactions with the neighbourhood.

The introductory literature review consists of three chapters. First, we present some basics of polycrystalline plasticity and texture modelling. The second chapter is an overview of significant experimental findings about grain splitting and neighbour interactions. Then, the theories available for simulating these two mechanisms are described and the choice made in this thesis is justified.

We then move on to the results, starting with the prediction of rolling textures. This is followed by the OIM study, to terminate with simulations of the build up of local orientation gradients using the LAMEL model and the FE model.
A piece of metal is normally made up of millions of crystallites arranged in an unknown, complex and irregular 3-dimensional aggregate. The only physically sound way to predict how the material responds to a given solicitation, is the so-called “micro-macro” approach. The philosophy of this approach is to consider a representative sample of the constituting crystallites, and to compute the polycrystal response as the average of all individual responses. It thus implies that some assumptions are made on how individual crystallites perceive the macroscopically exerted load, and that the behaviour of individual crystallites is correctly simulated. With the considerable increase of computing power, such micro-macro modelling has become much more promising than purely phenomenological models based on a macroscopic characterisation of the material anisotropy, e.g. the Hill model (1950).

This chapter aims at presenting fundamentals about polycrystal plasticity and texture modelling. A review will also be made of the historical developments that have convinced us of the necessity to incorporate grain interaction effects into micro-macro modelling. The first section describes the hypotheses shared by most polycrystal models, about how plastic deformation is accommodated at the level of individual crystallites. The second problem that is addressed is the description of the polycrystal in a manner convenient for simulations. Only then will the question of how macroscopic constraints apply to individual grains be considered, starting with classical theories that rely on an excessive idealisation of the aggregate's collective deformation.

In the present chapter, models are discussed from a purely theoretical viewpoint. Their performances in practical texture predictions will be evaluated in Chapter 4. Note also that complementary information about polycrystal plasticity theory and texture simulations can be found in the reference works by Aernoudt et al (1993), Hosford (1993) and Kocks et al (1998).
1 Single crystal plasticity

In many applications of polycrystal plasticity, elastic strains are much smaller than their plastic counterpart. This is certainly true for industrial rolling as plastic strains commonly reach values above 1.5 (which corresponds to 78% thickness reduction). In view of this and for the sake of simplicity, we neglect elastic strains and assume that the whole of the deformation is permanent.

At room temperature, cubic metals deform predominantly by dislocation slip along specific crystallographic planes and directions. In fcc metals, slip follows densely-packed {111} planes in <110> directions, defining 12 potential slip systems. In bcc metals, 24 slip systems are potentially active. The slip plane is {110} or {112} and the slip direction is <111>. The simultaneous activation of several slip systems gives the impression that slip can occur on all planes containing a <111> crystal direction, which is called “pencil glide”.

When a single crystal with an arbitrary (non-symmetric) lattice orientation is deformed in tension, dislocations move along only one slip system. It is the slip system with the largest “resolved shear stress” \( \tau_s \), i.e. the system in which the externally applied stress transforms into the largest shear stress, triggering dislocation motion.

\[
\tau_s = \sum_{i,j} \left( M_{ij}^s + M_{ji}^s \right) \sigma_{ij}
\]  

(1.1)

In this equation, \( M_{ij}^s \) is a geometrical factor that is equal to the product of two unit vectors, \( b_i^n \) and \( n_j^s \), where \( b_i^n \) is the slip direction and \( n_j^s \) is the slip plane normal. As \( b_i^n \) and \( n_j^s \) represent perpendicular directions, \( M_{11}^s + M_{22}^s + M_{33}^s = 0 \) and \( \tau_s \) depends solely on the deviatoric stress. In uniaxial tension, \( M_{11}^s \) is traditionally called the “Schmid factor” and reduces to \( \cos \Phi \cos \lambda \) where \( \Phi \) and \( \lambda \) are the angles that the tension direction makes with the slip plane normal and the slip direction, respectively.

\( ^{(1)} \) In fcc metals with low stacking fault energies (SFE), twinning is a second important deformation mechanism. Such materials are, however, not considered in the present thesis.
If the deformation is constrained, which is the case of single crystals compressed in a closed die as well as of individual grains in a polycrystal, “multislip” occurs. As plastic flow preserves volume, prescribing the deformation mode of a crystal implies, in general, the activation of five independent slip systems (not 6). A slip rate \( \dot{\gamma}_s \) on the \( s \)th slip system contributes to the local velocity gradient \( \mathbf{l}_{ij} \) with a simple shear rate equal to \( M_{ij}^s \dot{\gamma}_s \). However, the velocity gradient \( \mathbf{l}_{ij} \) can, in general, not be achieved by dislocation slip alone. This is easily seen when \( \mathbf{l}_{ij} \) is decomposed into its symmetrical \( d_{ij} \) and rotational \( \omega_{ij} \) parts (Eqs. 1.2-1.3). Supplementary to dislocation slip, a lattice rotation must ensure that material fibres aligned with the principal directions of deformation conserve this property after an infinitesimal deformation increment. The corresponding rotation rate, termed “lattice spin” and denoted \( \Omega_{ij}^\ell \), is responsible for texture development (further discussed in the next section).

\[
d_{ij} = \sum_s \frac{1}{2} (M_{ij}^s + M_{ji}^s) \dot{\gamma}_s
\]

\[
\omega_{ij} = \dot{\Omega}_{ij}^\ell + \sum_s \frac{1}{2} (M_{ij}^s - M_{ji}^s) \dot{\gamma}_s
\]

Although not all polycrystal plasticity models assume that the deformation of individual crystallites is known a priori, we now discuss two mathematical procedures for identifying, from a prescribed velocity gradient \( \mathbf{l}_{ij} \), which slip systems are active and what is the slip rate along each of them. In both cases, the \( \dot{\gamma}_s \) values are first derived from energy considerations, then \( \dot{\Omega}_{ij}^\ell \) is extracted from Eq. 1.3.

In the first procedure, the strain rate sensitivity of the material is considered to be negligible. Under this assumption, the “generalised Schmid law” states that slip occurs on all slip systems for which the resolved shear stress \( \tau \) reaches a critical value \( \tau_c \). The slip rates are obtained by minimising \( \dot{W} \), the plastic work rate dissipated internally by friction (Eq. 1.4), while satisfying the kinematical conditions (Eq. 1.2). This constrained minimisation is carried out most efficiently by relying on linear programming (Van Houtte, 1988).

\[
\dot{W} = \sum_s \tau_s^c |\dot{\gamma}_s| = \text{Min}
\]
It is important to note that the minimum dissipated energy $W$ is a function of the crystal orientation. A crystal may thus, based only on its orientation, be “harder” than another in the sense that its deformation implies more energy to be spent. This orientation effect can be characterised by the “Taylor factor” $M$ that is defined as

$$M = \frac{\sum |\dot{\gamma}_s|}{d_{eq}} = \frac{W}{\tau^c d_{eq}} = \frac{\sigma_{ij} \cdot d_{ij}}{\tau^c d_{eq}}$$  \hspace{1cm} (1.5)$$

where $d_{eq}$ is the equivalent velocity gradient. In this, it is assumed that all $\tau^c_s$ are equal. This equation shows that deforming a crystal with a high Taylor factor necessitates a larger deviatoric stress and gives rise to more dislocation slip, in total, on all slip systems. For example, in an aggregate with random texture subjected to plane strain compression, the grain Taylor factor $M$ varies between 1.84 and 4.22 for fcc slip, and between 1.78 and 3.71 for bcc slip. The Taylor factor is the origin of why a polycrystal’s overall strength depends on the global texture, and why metal plates that bear a strong texture are so anisotropic.

Another remark that should be made at this stage concerns the “Taylor ambiguity”. If the resistance to slip (i.e. $\tau^c_s$) is assumed to be identical in all slip systems, which is the case in the present work (1), the constrained minimisation of the plastic work does not yield a unique solution. One way to demonstrate this is to construct the single crystal yield locus (Fig. 1.1a) that is defined in the 5-dimensional deviatoric stress space by the conditions

$$-\tau^c_s \leq M_{ij} \cdot \sigma_{ij} \leq \tau^c_s \hspace{1cm} s = 1..n$$ \hspace{1cm} (1.6)$$

where $n$ is the number of potential slip systems. Applying the maximum work principle, Bishop and Hill (1951) remarked that most deformation modes are achieved at corners of this sharp-edged yield locus. Due to the symmetry of e.g. fcc lattices, the yield locus corners are not the intersection of 5, but rather of 6 or 8 hyperplanes corresponding to situations where 6 or 8 slip systems are equivalently stressed. As 5 independent systems suffice to accommodate $d_{ij}$, the

---

(1) In the real material, the $\tau^c_s$ values evolve during deformation due to dislocation interactions. In general, some “latent hardening” is observed: the resistance against slip increases faster for inactive slip systems. Such effects have, however, not been accounted for in the present thesis.
solution of the constrained minimisation (Eqs. 1.2, 1.4) is undetermined. These equally probable slip combinations accomplish the same strain with the same stress and the same Taylor factor, but a different lattice rotation. Therefore, a supplementary criterion must be applied in texture modelling, for selecting just one solution. This will be discussed more in detail in Chapter 4, where an original procedure will be proposed for solving this ambiguity.

![Diagram](image)

**Fig. 1.1** Illustration of a) the rate-independent, sharp-edged yield locus in deviatoric stress space, and b) the viscoplastic equipotential surface with rounded corners. c,d) Transition to another corner (i.e. another stress state) when the crystallite rotates.

The second procedure for computing the slip rates \( \dot{\gamma}_s \) takes account of the material strain rate sensitivity. In this case, the generalised Schmid law is not applicable and the concept of “yield locus” is meaningless. Instead, there is an exponential relationship between the slip rate \( \dot{\gamma}_s \) and the resolved shear stress \( \tau_s \) on each slip system:

\[
\dot{\gamma}_s = \dot{\gamma}_0 \left| \frac{\tau_s}{\tau_s^*} \right|^{\gamma_s^{-1}} \frac{\tau_s}{\tau_s^*},
\]

(1.7)
In this expression, $\dot{\gamma}_0$ is a material constant and $m$ is the “strain rate sensitivity” that is of the order of 0.01 (in fcc). By combining Eqs. 1.1, 1.2 and 1.7, the strain rate $d_{ij}$ is written in terms of the stress $\sigma_{ij}$. This permits the substitution of $d_{ij}$ in the expression of the dissipated plastic work (Eq. 1.8), defining a “viscoplastic equipotential surface” in (deviatoric) stress space:

$$P(\sigma_{ij}) = \sigma_{ij} d_{ij} = \text{constant.}$$  (1.8)

In fact, this equipotential surface resembles the yield locus of a rate-insensitive material, with the exception that the viscoplastic equipotential surface has rounded corners (Fig. 1.1b).

Under the assumption of rate-sensitivity, the ambiguity in the determination of the slip rates (“Taylor ambiguity”) is suppressed. The stress $\sigma_{ij}$ that corresponds to the prescribed strain rate $D_{ij}$ is determined by solving a set of five non-linear equations:

$$\frac{\partial P(\sigma_{ij})}{\partial \sigma_{ij}} = D_{ij}. \quad (1.9)$$

The slip rates $\dot{\gamma}_{s}$ are then obtained from $\sigma_{ij}$ using Eqs. 1.1 and 1.7. In practice, the solution of the viscoplastic calculation, amounts to distributing dislocation slip among all slip systems recognised as equivalently stressed by the former procedure. This is, a priori, in disagreement with the experimental observation that slip seems to be concentrated on one or two slip systems. To overcome this, strain rate dependency is often associated with a latent-hardening law that increases the $\tau_{c}$ values on less active slip systems, making them even less favourable for slip.

Strain rate dependent solutions are frequently chosen in finite element simulations for their mathematical convenience (Asaro and Needleman, 1985). However, the method may give rise to convergence problems in “relaxed constraints” Taylor models because these imply stress states that lie on edges or on facets of the yield locus (or equipotential surface) rather than corners. This is to be further discussed in Chapter 3.

Although it is clear that the real material is strain rate sensitive, one should not conclude that the second method for calculating the slips is more physically sound. It is possible that the Taylor ambiguity (predicted only by the first mathematical method) exists in the real material and that the choice among equally-stressed slip systems is dictated by some, here neglected, stochastic
parameter. Consequently, two grains with the same initial orientation and subjected to the same deformation could undergo different lattice rotations. The Taylor ambiguity could also be a source of grain subdivision, if different regions of a grain would select different slip combinations among the equally-stressed systems.

Another fundamental difference between the two methods appears if we analyse the rotation of a crystal during deformation. It is clear from their definitions that the yield locus and the equipotential surface rotate accordingly, with respect to the macroscopic loading axes. In order to maintain the normality of the strain rate tensor to the hypersurface, the stress must, at some stage, jump from one corner solution to another (Fig. 1.1c,d). Applying the “strain rate independent” method, we observe an abrupt change of the stress, the choice of activated slip systems and the Taylor factor. In the viscoplastic method, however, the yield locus is rounded off and a smoother transition occurs. In the real material, the transition is certainly not instantaneous but it could be fast enough to induce some instability such as strain localisation or grain subdivision. It is thus important not to omit the potential effects of these rapid transitions.

2 Statistical description of a polycrystal – Characterisation of texture

In the introduction, it is suggested that the crystallite aggregate constituting a metal component is too complex to be fully characterised. Only a statistical description of the aggregate, restricted to the most relevant material parameters, can reasonably be used as input for polycrystal plasticity simulations.

The deformation of a grain, under prescribed macroscopic constraints, is likely to depend on many characteristics of the aggregate in which the grain is embedded. Examples of potentially influential parameters are the size, shape and lattice orientation of the grain and of its neighbours, their topological arrangement, the presence of impurities/precipitates, and the history of deformation (pre-strain/residual stresses). Most of this information can be provided by modern experimental techniques. However, this sometimes implies a destruction of the sample by serial sectioning (Chapter 2), and, more importantly, not all parameters are equally useful.
Many plasticity models oversimplify reality by considering that the deformation and stress within a grain depend mainly, and sometimes even exclusively, on the local lattice orientation. In such models, texture is the only relevant material parameter and the polycrystal is fully described by its crystallographic orientation distribution function (ODF). The latter is denoted \( f(g) \) and indicates the volume fraction of crystallites bearing an orientation that is within the element \( dg \) around \( g \) in orientation space. Another interpretation is that grains with the orientation \( g \) are \( f(g) \) times more frequent than if the material had a “random texture” (i.e. if all orientations were equally probable).

In this work, we follow the convention of Bunge (1982) who proposed to write \( g \) in terms of Euler angles: the angles of three constitutive rotations bringing the reference “sample frame” on a “crystal frame” with axes parallel to \(<100>\) directions of the cubic lattice. As there are 24 equivalent definitions of the (right-handed!) crystal frame in a cubic lattice, any orientation \( g \) is characterised by 24 equivalent sets of Euler angles.\(^{(1)}\)

Plastic deformation of polycrystalline materials never happens without a sharpening of the crystallographic texture. To understand this, one should remember from Section 1 that only some special, “stable” lattice orientations allow accommodating a prescribed shape change without a superimposed rotation of the crystal lattice. In all other crystallites/grains, the lattice rotation remains effective until these grains have themselves reached a stable orientation. The proportion of grains having a stable orientation thus increases progressively with strain while all other orientations become rare.

When the deformation process bears some symmetry, the latter is gradually forced upon the developing texture. Rolling textures, for example, have an orthorombic symmetry because lattice orientations that are symmetric relative to the rolling direction (RD), the transverse direction (TD) or the normal direction (ND), have an equal chance to appear during deformation (Fig. 1.2). Such symmetry (not to be confounded with the crystal symmetry) is of statistical nature, and it is called “sample symmetry”. Actually, for rolling, the orthorombic sample symmetry is attained only in the centre of the plate where plane strain deformation is closely approached. It does not apply to the thin

\(^{(1)}\) In rolled samples, crystal orientations can also be characterised by the well-known Miller indices \([hkl]<uvw>\), representing the crystal directions that are aligned, respectively, with the normal direction and with the rolling direction (see Fig. 1.2).
layers in contact with the mills where friction and tool geometry cause shear. Furthermore, a perfect sample symmetry is achieved only when the initial texture has at least the same symmetry-level (or is random). In this work, only orthorombic rolling textures are considered.

Fig. 1.2 Definition of the reference sample axes in a rolled plate. Within the shaded zone, the material undergoes orthorombic plane strain compression (PSC).

By implementing the “crystal” and “sample” symmetries into the formulation, the ODF can be characterised with a minimum number of parameters:

$$ f(g) = \sum_{l=1}^{M} \sum_{\mu=1}^{N} \sum_{\nu=1}^{N} C_{l}^{\mu\nu} T_{l}^{\mu\nu}(g) $$

(1.10)

In this expression, $T^{\mu\nu}(g)$ are generalised spherical harmonic functions with built-in symmetries (Bunge, 1982), whereas the series coefficients $C^{\mu\nu}$ differ from one texture to another. In order to describe the texture of a given plate, the even $C^{\mu\nu}$ coefficients can be derived from the inversion of 4 pole figures (Van Houtte, 1995a), and the odd $C^{\mu\nu}$ coefficients can be computed by eliminating the negative “ghost” peaks from the ODF (Van Houtte, 1991).

However, such formulation of the ODF is not convenient for micro-macro simulations, which are based on a prediction of the behaviour of individual grains. Mathematical methods have thus been developed to discretise $f(g)$ into a set of grain orientations that are statistically representative of the overall texture (Toth and Van Houtte, 1992). Obviously, the number of discrete orientations (number of grains) to be used determines the computing time necessary for the simulation. As further discussed in Chapter 4, this number depends on the strength of the input texture and on the symmetry of macroscopic constraints.
At the end of a texture simulation, one has to recalculate the continuous ODF from the discrete set of predicted grain orientations. Here also, the harmonic series formulation is convenient: an analytical expression is available for generating such ODF by superposing spherical gaussian distributions in Euler space (Bunge, 1982). This analytical expression is also necessary when a texture is to be generated from local orientation measurements, for example by orientation imaging microscopy (OIM). This is the case of some experimental textures used as reference for the simulations in Chapter 4.

Note that another advantage of the series expansions is that they are extremely powerful for averaging orientation-dependent material properties (e.g. the Taylor factor under a prescribed deformation mode) over a polycrystal bearing texture (Bunge, 1982).

3 Classical theories of polycrystal plasticity

The role of polycrystal plasticity theories is to estimate how mechanical constraints applied at a polycrystal’s outer surface are distributed among the constituting crystallites. The same problem is encountered when studying polycrystal elasticity, or the deformation of multiphase materials (such as composite materials). In all cases, the solution is known to lie somewhere between the assumption of a homogeneous stress, and that of a homogeneous velocity gradient throughout the aggregate. These two extremes are termed, respectively, “lower” and “upper” bound solutions in reference to the associated deformation energy. In polycrystalline elasticity, the experimentally observed macroscopic response can often be closely estimated by taking the arithmetic average of the Voigt (upper) and Reuss (lower) predictions. This does however not apply to plasticity.

It is Sachs (1928) who first proposed a model for polycrystalline plasticity by supposing that all grains within a polycrystal are subjected to the macroscopic stress mode and that they deform by single slip similarly to unconstrained single crystals. Under this assumption, grains with distinct lattice orientations activate a different slip system (Eq. 1.1). Adjacent grains deform independently, leading to unrealistic overlaps and gaps at grain boundaries.

From the pioneer works of Taylor (1938), we know that the “upper-bound assumption” yields improved predictions of polycrystal stress-strain curves and texture evolution (Kocks, 1970). According to Taylor, each grain activates 5
slip systems so as to accommodate the macroscopically imposed velocity gradient while dissipating minimal energy by internal friction. Independent of the method used for calculating these slips (presented in the preceding section), the stress exerted in the grain is fixed and it is different in grains having different orientations. The Taylor hypothesis thus violates stress equilibrium at grain boundaries and is as unrealistic as Sachs’ idea although the deformation textures predicted by the Taylor model are generally closer to experiment (see Chapter 4).

In fact, even a solution for which deformation and stress differ from grain to grain but are homogeneous within each of them, would not fulfill stress equilibrium and strain compatibility. In the real aggregate, grains have so many direct neighbours that only strain and stress fields, which are heterogeneous inside the grains, can satisfy the interaction constraints. Analysing such stress and deformation fields is possible with finite element (FE) models relying on a fine discretisation of the grain volume (Chapter 3). These models are, however, too heavy for most practical case-studies, which justifies the development of less elaborated models still considering that the orientation, the velocity gradient and the stress are uniform within each grain. Some examples of the latter models are now presented.

In “relaxed constraints” (RC) models (Honneff and Mecking, 1978; Kocks and Chandra, 1982), the assumption of a uniform deformation throughout the aggregate is partly abandoned based on grain-shape considerations. These models have for example been applied to rolled materials where grains are flattened and a significant proportion of the total grain-boundary area lays parallel to the rolling plane. Along such boundaries, geometrical compatibility is not hindered by heterogeneities in the $l_{13}$ and $l_{23}$ shear deformations (where RD=1, TD=2 and ND=3). One may thus imagine that, in the real material, the $l_{13}$ and $l_{23}$ velocity gradient components are constrained only in the close neighbourhood of boundaries inclined to the rolling plane (Fig. 1.3). The RC “pancake” model (Van Houtte, 1982) proposes to neglect these small boundary regions and to allow free variations of $l_{13}$ and $l_{23}$ from grain to grain. In comparison with the Taylor “full constraints” (FC) model, the RC pancake model thus introduces two degrees of freedom in the plastic work minimisation (if $l_{13}$ and $l_{23}$ are relaxed, $d_{13}$ and $d_{23}$ are also relaxed). Consequently, only 3 independent slip systems need to be activated to fulfil the 3 remaining constraints. Moreover, as some components of $d_{ij}$ are free during the plastic-
work minimisation, the associated stress components $\sigma_{ij}$ are implicitly set to zero (see detailed mathematical proof by Van Houtte (1988)). At least for these components, stress equilibrium is now satisfied at grain boundaries. Finally, it is noteworthy that original RC theories, such as the pancake model, do not explicitly require that the average grain deformation is equal to the macroscopically exerted deformation. However, since RC theories predict opposite relaxations in grains with mirror lattice orientations (relative to the sample axes), deviations with regard to the imposed $l_{ij}$ are statistically cancelled out over any set of grains bearing a symmetrical texture.

After deformation:

Various authors proposed improvements of the RC Taylor theories. In the “continuous constraints model” by Fortunier and Driver (1987a), grains follow strain paths that are intermediate between FC and RC theories. The local deformation is calculated by minimising the change in plastic work rate ($\dot{W}$) which results from hardening of the slip systems as well as hardening or softening due to lattice reorientation and to interaction of the grain with its surrounding. The latter interaction is evaluated using a “self-consistent” or “autocoherent” scheme similarly to what is done in the models proposed by Lebensohn and Tomé (1993) and by Van Houtte and Rabet (1997). The assumption common to such theories is that each grain can be seen as an ellipsoidal inclusion embedded in a “homogeneous equivalent medium” (HEM) bearing the polycrystal macroscopic properties. The overall strain is distributed
over the aggregate based on the Taylor factor and on the relative anisotropy of each grain compared to the matrix. The interaction equations also determine the local skew-symmetric part of \( l_{ij} \), i.e. the rigid rotation of the ellipsoid. Rotational constraints are null for spherical inclusions, but increase as ellipsoids become pancaked (Van Houtte, 1995b). Eshelby (1957) demonstrated that, if the inclusion is ellipsoidal and if the HEM has linear properties, continuity and stress equilibrium can indeed be fulfilled with uniform stress and deformation inside the inclusion. However, in the real material, the grain surrounding is obviously heterogeneous (as neighbours have different lattice orientations) and the stress-strain relationship is non-linear. Self-consistent theories thus also lead to an oversimplification.

Mathur et al (1990) propose another interesting compromise between RC and FC theories. They consider that the percentage of grains submitted to relaxed constraints must increase continuously as the average grain shape evolves from equiaxed to pancaked. Their model is not restricted to rolling and plane strain compression. The plane in which grains undergo heterogeneous shears is not necessarily the rolling plane: it is the plane normal to the direction of the most negative principal strain \(^{(1)}\). Furthermore, in the formulation of Mathur et al (1990), \( \sigma_{13} \) and \( \sigma_{23} \) are not set to zero like in the pancake model, but they have a uniform value that is determined by minimising the dissipated energy simultaneously in all grains undergoing relaxed constraints. The model was applied to the prediction of through-thickness texture gradients in rolled plates undergoing redundant shear as well as friction at the rolls. Chastel and Dawson (1993) generalise the idea of Mathur et al (1990) by allowing all \( d_{ij} \) components to differ from grain to grain. This is necessary in lattice structures with few available slip systems (e.g. hcp) because a uniform deformation cannot always be achieved. In the Chastel and Dawson (1993) model, the stress mode is assumed to be uniform over the polycrystal but, instead of being prescribed like in the Sachs model, it is obtained by imposing that the average \( d_{ij} \) value is equal to the macroscopically exerted strain rate. The local skew-symmetric part of \( l_{ij} \) (i.e. \( \omega_{ij} \)) seems to be such that the principal directions of the local and of the macroscopic deformation tensors remain aligned with one another.

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\(^{(1)}\) More precisely: the average grain shape is computed by following the rotation and the stretch of a representative ellipsoid undergoing the macroscopic deformation. The plane for shear relaxation is normal to the shortest diameter of the ellipsoid.
Conclusion - How can classical theories of polycrystalline plasticity be improved?

In this chapter, several theories have been described for performing the macro-to-micro transition that distributes strain and stress among the constituents of a polycrystal. All these theories make two oversimplifications relative to the real micromechanics:

1° Strain, stress and lattice orientation are assumed to be homogeneous within individual grains.

2° Potential effects of the grain arrangement topology are disregarded: any two grains having a common initial orientation are predicted to undergo the exact same deformation (1).

As commented in the previous section, these simplifications make it impossible to ensure strain compatibility and stress equilibrium at grain boundaries. It is thus clear, already from a theoretical reasoning, that grains of the real material interact with their direct neighbours and have non-uniform strain, stress and orientation. In the next chapter, microstructural observations will demonstrate that such heterogeneities appear in the form of grain-scale orientation gradients as well as a subdivision of the grain into volumes undergoing distinct deformation. We will see that grain interactions are not the unique driving force for grain subdivision. We will also try to assess whether subdivision and/or direct-neighbour grain interactions have a significant influence on texture evolution.

(1) In self-consistent theories and in the model proposed by Mathur et al (1990), the deformation of a grain is influenced by the global texture (disregarding the spatial arrangement of the grains). In all other models, the local deformation is solely dependent on the grain orientation.
According to the plasticity theories presented in the first chapter, the deformation of a polycrystal can be achieved by a flow of dislocations gliding along particular crystallographic planes of the constituting grains. In the real material, things are actually more complex because dislocations interact with one another, and can be immobilised in the bulk of a grain instead of carrying shear throughout the whole grain volume (i.e. not all mobile dislocations reach the grain boundary). Dislocations appear to organise themselves into characteristic patterns, subdividing the grains on a much smaller length-scale than expected from the gradients caused by interactions with the grain surrounding. Microstructural observations tend to indicate that dislocation patterning augments the intra-granular heterogeneity of strain, stress and lattice orientation. Dislocation patterning is also the principal source of hardening in metals, and it has significant effects on the evolution of texture and on the macroscopic flow anisotropy.

This second chapter presents a selection of results from the abundant literature in the field of deformation microstructures. The aim is to gather experimental information that can be relevant for the incorporation of grain interactions and grain fragmentation in plasticity modelling. More specifically, the focus is set on microstructural hints about what triggers subdivision and about the influence of grain splitting on texture evolution. Due to its relevance in the present thesis, one section is devoted to the experimental investigation of grain interaction effects on the local plastic deformation and on the developing substructure.

In the specialised literature, experimental observation and theoretical interpretation can sometimes hardly be dissociated. The present chapter is, however, as much as possible restricted to experimental facts. A discussion of
existing theories about the driving forces of subdivision and their implementation in texture simulations is postponed to Chapter 3.

Literature results, which are referred to, have been obtained on cubic metals deformed mainly by rolling. Microstructural studies are often carried out on rolled samples because, besides the obvious industrial relevance of rolling, these samples may be highly strained without failure. Furthermore, observations in the “long transverse” section (i.e. section containing RD and ND) yield a lot of information about the grain splitting process.

1 Characterisation of deformation microstructures in rolled cubic metals

In this section, an inventory is made of grain subdivision patterns that appear successively with increasing rolling strain. In each case, we try to determine to which extent local strains are heterogeneous, and how large the thereby created misorientations are. We will therefore rely on various observation techniques:

- The local heterogeneity of deformation is observable only on free sample surfaces where slip lines indicate the traces of active slip systems, and where the displacement of markings, such as micro-hardness indentations, can be followed.

- The non-uniformity of lattice orientation is most accurately revealed by analysing electron diffraction patterns. Recent developments in both scanning- and transmission electron microscopy (SEM and TEM) allow an automatic orientation mapping of sample surfaces. Orientation mapping in the SEM has been applied in this work and will be discussed in detail in Chapter 5. If large misorientations occur within a grain, this can also be detected using optical microscopy with polarised light.

- However, at the onset of subdivision, the heterogeneity of deformation and orientation is too small to be identified by any existing technique. At this stage, one has no alternative but to analyse the formation of dislocation structures on TEM images.

A surprising phenomenon is that subdivision patterns encountered in single crystal experiments are quite similar to those observed in polycrystalline
Chapter 2 Experimental observations

Contrarily to individual grains imbedded in a polycrystal, the deformation of a single crystal is not subjected to interactions with surrounding grains. On the other hand, strain and stress heterogeneities that arise from friction with the die or the rolls can propagate through the whole single crystal volume, which is obviously not the case for grains in the bulk of a polycrystal. Nevertheless, the resemblance of the dislocation structures in single- and polycrystal experiments justifies the use of single crystals to investigate lattice orientation effects on subdivision patterns.

1.1 Lowest scale subdivision (3D cell array)

The first microstructural feature that appears during plastic straining of both bcc metals and high stacking fault energy (SFE) fcc metals is the arrangement of dislocations in a three-dimensional cellular array (e.g. Gil Sevillano et al, 1980). The micrometer-sized volumes that are formed have a much lower dislocation content than the boundaries around them. This enables their observation in the transmission electron microscope (TEM).

Cell boundaries have no directionality (see Fig. 2.2), which seems to indicate that the constituting dislocations were incidentally trapped in this configuration as a result of their interactions. For this reason, cell boundaries are often called “incidental boundaries”. Also, the development of such tri-dimensional configurations is an indication that deformation is accommodated by slip on a variety of slip systems, i.e. “polyslip state” (as predicted by the Taylor model). The creation of the cellular array seems to also necessitate cross-slip since it is encountered in “wavy glide materials” but not in low SFE metals in which the cellular array is replaced by a more diffuse “Taylor lattice” (Bay et al, 1990). Another peculiarity of low SFE metals is, of course, twinning (Gil Sevillano et al, 1980) but this will not be treated here.

The misorientation between adjacent cells is of the order of 0.3-1.5° and the cell diameter is around 1µm. Looking more in detail, it appears that the misorientation increases with increasing strain (proportionally to \( \varepsilon_{eq}^{1/2} \)) whereas the cell size decreases (Hughes and Godfrey, 1998). However, because misorientations remain low (\( \theta_{avg} \sim 1° \) at \( \varepsilon_{eq} = 1 \)) and because randomly oriented cell boundaries can only harden all slip systems in the same way, it is expected that this subdivision type has a negligible effect on texture evolution.
1.2 Low and medium strain microstructures (ε<1.0)

When the plate thickness has been reduced at least 10-15%, a second type of subdivision occurs with a somewhat larger scale than the cell size. Grains are subdivided into parallelogram-shaped volumes that are 1-3µm thick and more than 10µm long when observed in the longitudinal plate section (section containing RD and ND). Depending on the material, there are actually two distinct mechanisms by which this meso-scale subdivision takes place.

1.2.1 Subdivision by "microbands" (MBs)

The term “microband” was first proposed by Malin and Hatherly (1979) for describing a new microstructural feature in cold rolled copper. Performing transmission electron microscopy in RD-ND sections of the plate, microbands appear as thin (0.2-0.4µm thick) plane regions bounded by two parallel dislocation walls (Fig. 2.1). Such microbands (MBs) are several 10µm long and seem to be formed parallel to the most stressed {111} slip plane. The enclosed volume has a high dislocation content and is only slightly misoriented with regard to the surrounding matrix. Furthermore, MBs form slip bands at free surfaces due to the localized shear within them. This was demonstrated by careful TEM inspection of surface replicas from pre-polished samples revealing shear offsets when MBs crossed surface markings (Fig. 2.1). According to Malin and Hatherly (1979), the localized shear inside MBs could account for the whole of the macroscopically exerted deformation, at moderate rolling reductions. However, MBs are not fully equivalent to “shear bands” (1) because MBs are confined to single grains: they never cut through grain boundaries.

Subsequent studies on rolled copper corroborate most of the observations made by Malin and Hatherly (1979). Torrealda and Gil Sevillano (1982) do, however, not attribute microband creation to localized shear. According to them, shear strain localization would become evident only after some critical strain (ε~0.3). Leffers et al (1991) consider that not all grains deform predominantly by “single slip” along MBs: geometrical compatibility must be ensured by polyslip in the neighbouring grains. In any case, as reported by Nes et al (1985), the formation of MBs in rolled copper is a transient stage of very heterogeneous slip that appears due to an instability of the cell structure and that

(1) To be presented in the section about the "high-strain microstructures".
disappears at high strains because in-grain misorientations impede long-range crystallographic slip. The same authors state that microband formation relies on the availability of redundant dislocations and that it is therefore not encountered in high purity aluminium where, according to the authors, dynamic recrystallisation occurs.

Microbands are also observed in cold rolled iron and steel (Aghan and Nutting, 1980; Österle et al, 1983; Roven and Nes, 1984; Inagaki, 1990; Akbari et al, 1997). Many similarities are found with the copper case. In bcc of course, active slip planes along which MBs can form are \{110\}, not \{111\}. Another point that is stressed here, is the observation of steps when MBs meet grain boundaries. According to Inagaki (1990), these steps constitute stress concentrations and could be the origin of MBs rather than a consequence of the localised shear within the band.

In many of these studies performed on copper (Nes et al, 1985; Leffers et al, 1991) or steel (Akbari et al, 1997; Inagaki, 1990), it is also reported that two families of crossing MBs coexist. These authors also underline the tendency of MBs to bear a macroscopic orientation close to the plane with maximum shear stress. Assuming a perfect plane strain deformation, this maximum shear stress plane is parallel to TD and makes an angle of $+45^\circ$ or $-45^\circ$ with respect to RD.

By appearing at regular intervals (1-3µm) over the grain area, MBs delineate banded volumes that undergo little deformation (which is compensated by localised shear within MBs) and that do not have the tendency...
to develop misorientations with one another. This does not mean that microband formation has no effect on texture evolution. Österle et al. (1983) observed that texture evolution is slower during the strain range coinciding with microband formation. These authors remarked a similar reduction of the texture evolution rate, at high strains when shear bands start to form. During the microband transient stage, they suggest to replace the Taylor hypothesis of a homogeneous strain by a model for shear band deformation (Van Houtte et al., 1979).

1.2.2 Subdivision into “cell blocks” (CBs)

A material in which dislocation structures have been extensively studied in the last decades is rolled aluminium (reviews by Bay et al. (1992) and Hansen and Juul Jensen (1999)). In an aluminium plate, grains are subdivided by extended planar dislocation walls that delineate “cell blocks” (CBs) \(^{(1)}\). CBs are 1-2 µm thick, they are parallelogram-shaped and they contain cells. The planar CB boundaries are termed “dense dislocation wall” (DDWs) when the boundary is single, and “microband” when it is double (Fig. 2.2). Similarly to the MBs observed in copper, these dislocation boundaries are formed parallel to the most stressed \{111\} plane and they later adopt the macroscopic directionality of the maximum shear plane.

Although they have received the same name, there is a fundamental difference between, on the one hand, “microbands” separating CBs in aluminium and, on the other hand, “microbands” in copper or steel. In aluminium, there is no concentrated shear within MBs and the whole deformation takes place in the matrix, i.e. in the CBs. The latter statement is easily verified by the absence of shear offsets at intersections of two families of MBs in aluminium, contrarily to the copper case (Leffers et al., 1991). The latter authors proposed a different terminology “1\(^{\text{st}}\) generation MBs” would not contain any localised shear, whereas “2\(^{\text{nd}}\) generation MBs” would.

The formation of CBs seems to be a consequence of the heterogeneity of dislocation slip within the grains. Each CB is constituted of cells among which dislocation slip and deformation are homogeneous but different from the surrounding. DDWs and 1\(^{\text{st}}\) generation MBs thus have the function to separate

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\(^{(1)}\) Cell-blocks (CBs) have also been observed in different aluminium alloys as well as in cold rolled nickel (Bay et al., 1992).
volumes with different slip patterns and between which a lattice misorientation develops. They are, for this reason, termed “geometrically necessary boundaries” (GNBs) as opposed to the “incidental boundaries” between the cells. It is further often stated that each CB deforms with less than 5 active slip systems and that the macroscopic deformation can be accommodated only collectively, at the grain level. Theoretically, this permits a reduction of the plastic work while maintaining compatibility at grain boundaries.

Misorientations between CBs can be as high as 15° after 40% rolling reduction (Bay et al, 1992). Subdivision into CBs may thus have a significant effect on texture evolution. Also, the extent of CB subdivision appears to be dependent on the grain orientation. This has been investigated by Liu et al (1998a) on commercial purity (AA1050) polycrystalline aluminium. The authors found CBs with higher misorientations in grains oriented near the cube orientation $\{001\}<100>$. Other differences were observed concerning the planarity of the CB structure and the crystallographic character of the walls.

![Fig. 2.2](image-url)  
**Fig. 2.2**  a) Schematic representation of the subdivision into cell blocks at low strain (Bay et al, 1992)). b) TEM image of a ~40% cold rolled aluminium sheet (courtesy X. Huang, Risø National Lab.). In the latter image, each CB contains only one cell through its thickness, contrarily to the drawing in a).
1.2.3 Comments on the macroscopic directionality of microband and cell block substructures

Although the subdivision by MBs (in copper, iron and steel) and the subdivision into CBs (in aluminium and nickel) appear as two distinct mechanisms, the associated dislocation patterns have a very similar directionality with regard, first, to the lattice orientation, then, to the sample axes. In all these materials, grains are cut-through by extended planar dislocation sheets that are initially formed parallel to the most stressed slip system. With increasing strain, these sheets tend to become aligned with the macroscopically most stressed plane, i.e. the “maximum shear” plane. Assuming that ideal plane strain compression (PSC) is approached during rolling, the maximum shear plane is tilted of $+45^\circ$ or $-45^\circ$ relative to the rolling plane and it contains the transverse direction (TD). The same directionality has been observed in aluminium deformed in tension (boundaries at 45° to the tension direction), nickel deformed in torsion (boundaries parallel and perpendicular to the shearing plane) and steel deformed in tension or simple shear. For more information, the reader is referred to Winther et al (2000), Hughes and Hansen (1991), and Rauch and Thuillier (1994), respectively.

Neither the creation of these extended dislocation sheets, nor their subsequent re-orientation during deformation is well understood. Concerning their creation, it may be noted that the immobilisation of dislocations along planar walls parallel to the most stressed slip plane creates obstacle-free channels for other dislocations carrying deformation along this slip system. This argument takes however no account of the micro-mechanical function of the walls (localised slip / geometrically necessary boundary). Other explanations have been proposed e.g. by Torrealda and Gil Sevillano (1982) in copper. The subsequent re-orientation of the walls close to the maximum shear plane is also mysterious. For some unknown reason, these extended planar dislocation walls maintain a macroscopic orientation that is not bound to the lattice and that also disobeys the rotation towards the rolling plane expected from pure kinematics (Fig. 2.3). This inconsistency has been outlined by Nes et al (1985) and Christoffersen and Leffers (1998) for copper, and by Bay et al (1992) for aluminium. One explanation could be that the walls recorded after rolling 40% are not those that were observed at, say, 15% reduction. The substructure would thus constantly be destroyed and replaced by a new one with a constant directionality. Another solution is that the walls rotate backward relative to what
is imposed by PSC (Christoffersen and Leffers, 1998). Pantleon and Hansen (1998) simulate this re-alignment of the walls based on a minimisation of the dislocation interaction energy (see the LEDS theory in Chapter 3).

![Fig. 2.3 Rotation of a material line as expected from kinematics.](image)

Finally, we wish to comment on the many figures presented in literature wherein these extended dislocation sheets have, at the same time, a macroscopic and a crystallographic character. Regarding this, it must be noted that the maximum shear plane coincides with an active slip plane only for some special lattice orientations. This is illustrated in Fig. 2.4, giving the orientation range for which a potentially active slip system (\{111\} plane for fcc and \{110\} plane for bcc) is found within 5°, 10° or 15° of the maximum shear planes. This 5°-15° tolerance is used to reflect the likely deviations from PSC due to grain interactions and the limited resolution of the experimental observations reported.

![Fig. 2.4 Illustration of the probability that the maximum shear plane (plane inclined at +/-45° to the rolling plane around TD) coincides approximately with a slip plane: a) in fcc and b) in bcc. The contours indicate tolerances of 5°, 10° and 15°.](image)
These ODFs show that only a small proportion of the orientation space is such that either a \{111\} or a \{110\} crystallographic plane coincides approximately with a maximum shear plane under PSC. Among the texture components that are produced during rolling of fcc metals (to be discussed in Chapter 4), only \(S\) \{123\}<634> and \textit{copper} \{112\}<111> fulfil this condition. Among the orientations that are produced during rolling of bcc metals (also to be discussed in Chapter 4), only \(F\) \{111\}<112> is satisfactory.

\subsection*{1.2.4 Localised glide in aluminium crystals with specific orientations}

At rolling strains of ~1, strain localisation occurs in grains with specific orientations in aluminium (Driver et al, 1994; Godfrey et al 1998a). This localisation consists of 1-10µm thick sheared bands that are parallel to \{111\} slip planes. In crystals with \(S\) \{123\}<634> orientation, localised shear deforms the cell-block pattern into characteristic “S-bands” (Fig. 2.5). In crystals with \textit{copper} \{112\}<111> orientation, localisation rather appears as “micro-shear bands”. In both cases (and contrarily to the MBs in copper and steel), the present strain concentration is associated with large orientation gradients (Hughes and Hansen, 1997).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{s-bands.png}
\caption{S-bands in aluminium (courtesy X. Huang, Risø National Laboratory).}
\end{figure}
The two cited orientations are stable components of fcc rolling textures (Chapter 4). Another orientation that is stable with regard to texture evolution, brass \{110\}<112>, has been observed to maintain very homogeneous CB structure (Godfrey et al 1998b). On the other hand, the cube \{001\}<100> orientation that is an unstable texture component forms highly misoriented fragments similarly to the two first orientations cited. There seems, thus, to be no direct link between the resistance to strain localisation and the stability during texture development.

1.3 **Large strain microstructures (\(\varepsilon\geq 1.0\))**

1.3.1 **Deformation banding**

In all materials considered (copper, iron, steel, aluminium, nickel), the medium-strain substructure is only a transient that does not pertain to high strains. At rolling reductions larger than \(~50\)%, one observes a lamellar substructure that is aligned with the rolling plane (e.g. Aghan and Nutting, 1980; Hatherly, 1986). Comparing the thickness of the lamellas to the grain thickness expected after a given rolling reduction, it is evident that some subdivision occurred. Lee and Duggan (1993) reported that copper grains with original grain size 3000\(\mu\)m subdivided, on average, into 25 layers of different orientation after rolling 85%. In another plate, copper grains with original grain size 40\(\mu\)m formed an average of only 2.4 layers after the same reduction. The orientations of some of these layers were twin-related but not all. The same authors also found lamellar subgrains parallel to the RD-ND plane. An example that they give is schematised in Fig. 2.6. It is a coarse copper grain subdividing into alternative bands of complementary brass orientation (110)[1 1 2] and (110)[1 1 2]. The latter pattern was also predicted by Aernoudt and Stüwe (1970) and will be further discussed together with the modelling results of this thesis.

The subdivision into this lamellar microstructure is attributed to “deformation banding”. This subdivision mechanism was first reported by Barrett (1939) who called “deformation bands”, regions of a grain that have distinct lattice orientations as a result of plastic deformation. These regions are separated by “transition bands” having a finite width (contrarily to grain boundaries) and across which the lattice orientation changes gradually. Often, alternative orientation changes are found across adjacent bands that are then termed “kink bands”.


Fig. 2.6 Subdivision of coarse grained copper into deformation bands perpendicular to TD and bearing alternating (1 1 0)[1 1 2] and (1 1 0)[ 1 1 2] orientations (from Lee and Duggan (1993)).

It is still unclear how the medium-strain regime with extended planar dislocation walls tilted at ~40° relative to the rolling plane, transforms into lamellar deformation banding at high strain. Contrarily to what was originally suggested the medium-strain bands do not rotate to the rolling plane simply due to the compressive strain (section 2.2.3). Some authors suggest that CBs and MBs are re-oriented parallel to the rolling plane due to shear localisation (S-bands, shear bands,…). However, according to other reports, deformation banding parallel to the rolling plane precedes shear localisation. Therefore, the lamellar deformation bands could actually be a new structure that is independent of the medium-strain dislocation structure.

Deformation banding has at least as strong an effect on texture as CB formation. It gives rise to high misorientations within the grains (Hughes and Hansen, 1997) and the extent of deformation banding is dependent on the original grain orientation. Studies have shown that grains with cube {001}<100> orientations were preferred sites for deformation banding (e.g.

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(1) At large strain, misorientations can become so large that it is impossible to tell whether two adjacent lamellas originate from a common parent grain.
Chapter 2 Experimental observations

Dillamore and Katoh, 1974). Hjelen et al (1991) and Liu and Hansen (1997) reported cumulative lattice misorientations in transition bands around axes near TD. This has been confirmed by single crystal experiments (Liu et al, 1998b; Godfrey et al, 1998a). In single crystal studies, the orientation of deformation bands is strongly influenced by macroscopic boundary conditions. When a single crystal with cube orientation is compressed in a channel die, DBs form almost parallel to the plane perpendicular to TD (Liu et al, 1998b). However, the same single crystal forms DBs parallel to the rolling plane when it is cold rolled (Liu and Hansen, 1998).

Finally, it must be mentioned that deformation banding receives particular attention because transition bands constitute recrystallisation nuclei during the annealing treatment after rolling (e.g. Hjelen et al, 1991; Engler, 1996).

1.3.2 Shear bands

Shear bands are macroscopic slip localisations that only occur after large rolling strains. Contrarily to “2nd generation MBs” in copper and steel (Section 1.2.1) and to S-bands (Section 1.2.4), shear bands extend over many grain diameters. Moreover, they have an orientation that is always macroscopic (no direct relation with a crystallographic plane): they are parallel to TD and tilted at ~35° to the rolling plane. The conditions for shear band formation have been theoretically investigated by Dillamore et al (1979) and by Van Houtte et al (1979).

Although shear bands do not divide the grains into highly misoriented fragments, they certainly have an effect on texture evolution. Indeed, concentrated shear within the band may substitute itself to plane strain compression in the matrix, leading to a slower texture development. This effect was studied by Österle et al (1983) as already discussed in section 1.2.1.
2 Experimental proofs of grain interaction effects

2.1 Effect of grain interactions on texture evolution

Even though it is clear from a theoretical reasoning that grains of a polycrystal must interact (see Chapter 1), finding experimental traces of the interaction is not an easy matter. For example, it is still impossible to evaluate in how much the lattice rotation of a grain imbedded in the bulk of a polycrystal depends on the orientation of its direct neighbours. Until now, orientation mapping can cover only the outer surface of a sample, not a section in the bulk. Final grain orientations can be recorded in cross-sections of the deformed sample but the initial orientations and the initial topology of the grains remain unknown. In the future, this crucial information may be provided by synchrotron X-ray diffraction across undeformed bulk samples. Juul Jensen and Poulsen (2000) are currently attempting this with, so far, a spatial resolution of $5 \times 5 \times 50 \mu m^3$ and an angular accuracy of $0.1^\circ$.

Two experimental techniques have been proposed for recording the deformation history of a set of interacting grains from two-dimensional orientation maps. On the one hand, Skalli et al (1985), Delaire et al (2000) and Bhattacharyya et al (in press) follow the deformation of a “multicrystal” made of a small set of coarse grains which extend up to the sample outer surface. On the other hand, Panchanadeeswaran et al (1996) mapped grain orientations in the ND-RD section of an aluminium sample split in two parts. The preliminarily inspected area was held in contact with its matching face on the other half of the split-sample, during channel-die compression. In such experiments, great care must be taken to avoid friction with the die or the rolls: Teflon films are therefore used as lubricant and hardness indentations serve to check the local deformation. Panchanadeeswaran et al (1996) and Bhattacharyya et al (in press) report that individual grains rotate towards stable texture components but not towards the components that are predicted by the Taylor FC model. They attribute this to grain interaction effects, based on the observation of significant divergences relative to the macroscopically imposed deformation. Skalli et al (1985) come, however, to the opposite conclusion: they follow the orientation path of 19 coarse grains in two rolled aluminium plates and find that grains having the same initial orientation but different neighbours rotate towards the
same end-orientation. The behaviour of the 19 grains is between the predictions of the FC and RC Taylor models, which is at the basis of the “continuous constraint model” (Chapter 1).

The latter experimental procedures are very promising. Tremendous effort is, however, still required to gather statistically reliable information. As discussed in Chapter 3, such studies can valuably be complemented by FE simulations.

2.2 Traces of grain interactions in the substructure

It is a widely-spread theoretical argument that strain and stress compatibility do not enforce the activation of 5 slip systems over entire grain volumes, but only close to boundaries and triple junctions (e.g. Kocks and Canova, 1981). Schematic drawings of the expected slip line pattern in surface grains (Fig. 2.7) are often shown but experimental results demonstrating this are not so frequent. In a review paper, Hansen (1985) provides evidence of “accommodating slip lines” extending from grain boundaries. The same author further shows that, when slip lines encounter a boundary, they can cause secondary slip or even penetrate a short distance into the neighbouring grain. The former observation is at the basis of the “modified Sachs model” by Leffers (1981) (Chapter 3).

Fig. 2.7 Number of activated slip systems within a grain (right), and slip lines as they would appear on a pre-polished free surface (left).

A TEM analysis by Liu and Hansen (1997) on cold rolled aluminium reveals perturbations of the dislocation structure in grain boundary regions.
Morphological differences in the dislocation structure are found not only with regard to the grain interior but also along the boundary. This indicates that different neighbouring grains have different effects. Note that these perturbations of the microstructure are found to correlate well with perturbations in lattice orientation and that the affected grain boundary regions can be up to 10\(\mu\)m thick in grains with an average diameter of 50\(\mu\)m.

Leffers and Christoffersen (1997) see, in the heterogeneity of subdivision patterns occurring in cold rolled copper, an indication of grain interaction effects. In such material, 50% of the grains develop a “high wall density” (HWD) structure consisting of two families of planar dislocation walls lying approximately at \(+\) and \(-45^\circ\) to the rolling plane and parallel to TD. According to the authors, there is no doubt that the formation of the HWD structure is dependent on the slip activity. However, no correlation is found between the crystallographic orientation of grains and the occurrence of the HWD structure. They conclude from this that the local slip activity is strongly influenced by grain interactions. Furthermore, as subgrain walls are not aligned with crystallographic planes (Christoffersen and Leffers, 1997), the significant scatter around the ideal macroscopic tilt of the walls (i.e. the maximum-shear plane under PSC) is an indicator of severe local deviations relative to the macroscopic deformation.

Always in copper but at higher strains, Duggan et al (1999) observe that deformation banding is influenced by the orientation of surrounding grains. The authors report that, without exception, subdivided grains are surrounded by grains of lower Taylor factor that do not split. If no such “softer” grains are present in the grain neighbourhood, deformation banding does not take place. Fortunier and Driver (1987) followed the deformation and the reorientation of 24 grains in a coarse-grained aluminium sample and they observed most extensive deformation banding in the “hardest” grain bearing a \{110\}<110> orientation. The interpretation of Duggan et al (1999) is that grains with high Taylor factor have only 2 or 3 systems favourably oriented for slip. During deformation banding, slip is restricted to these 2 or 3 systems (instead of 5). This saves energy on the condition that the heterogeneous deformation is accommodated by multislip in “softer” grains around. According to this interpretation, the slip pattern of homogeneously deforming “softer” grains is also very much dependent on their direct neighbourhood, i.e. on the orientation of the “hard” grain.
Hutchinson (1999) holds a similar reasoning in a review paper about deformation microstructures in steel plates: “hard” grains oriented along the $\gamma$-fibre (1) are subjected to intra-granular heterogeneities, whereas “soft” grains oriented along the $\alpha$-fibre (1) undergo inter-granular heterogeneities. To support this statement, the author first remarks that during rolling of steel, the energy stored within a grain (revealed by preferential etching or by the formation recrystallisation nuclei) is positively correlated with the grain Taylor factor. Then, he refers to microstructural studies (i) by Every and Hatherly (1974) revealing deformation banding and high misorientations in $\gamma$-fibre grains as opposed to homogeneously oriented cellular arrays in $\alpha$-fibre grains; and (ii) by Vanderschueren et al (1996) showing $\alpha$-fibre grains bent around a “hard” $\{011\}<011>$ grain having a “fish-bone” microstructure. According to Hutchinson (1999), the enhanced subdivision of $\gamma$-fibre grains is not subjected to the condition that the grain surrounding is soft. The high Taylor factor of $\gamma$-fibre grains is also indicative of a more abundant slip activity, which increases the chance for dislocation immobilisation (i.e. stored energy). Moreover, it is only when the Taylor factor for plane-strain deformation is high, that significant energy can be saved by localised shear. The latter argument is supported by the observation of coarser slip bands in such grains.

3 Conclusion

This chapter has shown that grain subdivision appears in various forms in cold rolled cubic metals. Two types of subdivision mechanism seem predominant: the localisation of shear deformation (copper MBs, S-bands, shear-bands), and the partitioning of strain among grain regions that might accommodate the macroscopic shape-change collectively (CBs, kink bands). The latter heterogeneously deforming regions are separated either by “smooth” orientation gradients (transition bands separating deformation bands), or by dislocation walls accommodating a “discrete” misorientation (DDWs and MBs that delineate CBs).

1 The $\alpha$- and $\gamma$- crystallographic fibres contain predominant texture components in rolled steels, as will be discussed in Chapter 4.
Although they are not as obvious as could have been expected from a theoretical reasoning, some effects of grain interaction on texture evolution and on the deformation microstructure are visible.

Most of the encountered subdivision types must have noticeable effect on texture evolution. This can be attributed to different factors: the development of an orientation spread within the grain, the localisation of strain within thin bands, and/or the orientation dependence of splitting. However, as most of the cited studies rely on high-resolution microscopy for observing the finest details of the dislocation structure, they could not cover sufficiently large areas to obtain statistically reliable quantitative information about the effect of in-grain heterogeneities on texture evolution. This is the aim of the OIM study performed in Chapter 4.

The next chapter describes existing theories for simulating grain interactions and grain subdivision. We can already guess from the complexity of the changing microstructure that not all features can be simulated with a single model.
CHAPTER 3: THEORIES ABOUT GRAIN INTERACTIONS AND GRAIN SUBDIVISION

A presentation is here given of models that aim to overcome the two main limitations of classical plasticity theories (Chapter 1): (i) the deformation of a grain should depend on the orientations and the topology of the surrounding grains, and (ii) strain, stress and orientation should be non-uniform within each grain. The first models considered are grain interaction models that still assume a uniform deformation within individual grains (no subdivision). Then, we move on to models simulating the development of in-grain heterogeneities, and we distinguish between models supposing that the heterogeneity is triggered solely by interactions with the grain neighbourhood, and models in which it is triggered by dislocation patterning. In the final discussion, we define the scope of the simulations and the experimental measurements to be performed in the second part of this thesis.

1 Modelling grain interactions with $N$-site polycrystal models

It is wrong to think that any two grains having a common initial orientation would always deform in the exact same way. Several experimental studies reported in Chapter 2 have shown that the deformation of a grain not solely depends on its own lattice orientation, but appears to be affected also by the topology and the orientations of the neighbouring grains. “$N$-site” plasticity theories take account of specific interactions between neighbours by solving the plasticity equations simultaneously for $N$ interacting grains.
1.1 The LAMEL model

The LAMEL model (Van Houtte et al, 1999) is a compromise between two of the classical theories presented in Chapter 1: the “full constraints” (FC) Taylor model and the relaxed constraints (RC) “pancake” model (Fig. 3.1). The LAMEL model assumes that, in a rolled material, grain interactions should predominantly take place across boundaries that are parallel to the rolling plane. The model simulates the co-operative deformation of two lamella-shaped grains separated by one such boundary. The two grains may undergo shear deformations parallel to the rolling plane. However, instead of being completely relaxed as for the pancake model, these shears are subjected to the condition that no grain boundary sliding occurs along the interface separating the grains. This means that the two grains deviate from the macroscopic deformation by exactly opposite shear deformations (Fig. 3.1).

In the LAMEL model, the slip activity is computed simultaneously for the two interacting grains. The slip rates and the shear relaxations are found by minimising the total internal plastic work rate

$$W_{TOT} = W_I + W_H = \sum_s \tau_{s}^{I} \dot{\gamma}_{s}^{I} + \sum_s \tau_{s}^{II} \dot{\gamma}_{s}^{II}$$

where the roman indices $I$ and $II$ refer to the two grains. The minimisation is performed while satisfying the following kinematical constraints

\begin{align*}
\text{Taylor FC} & \quad \text{LAMEL} & \quad \text{Tayl. RC - "Pancake"}
\end{align*}
\[ d_{ij}^I = \sum \frac{1}{2} \left( M_{ij}^I + M_{ji}^I \right) \gamma_s^I = D_{ij} + \dot{\gamma}_{ij}^L \] 

(3.2)

\[ d_{ij}^H = \sum \frac{1}{2} \left( M_{ij}^H + M_{ji}^H \right) \gamma_s^H = D_{ij} - \dot{\gamma}_{ij}^L \]

where \( D_{ij} \) is the macroscopic velocity gradient tensor, and \( \dot{\gamma}_{ij}^L = 0 \) except for \( ij = 13 \) and \( 23 \) \(^{(1)}\). These kinematical constraints represent 10 linear equations with \( 2n + 2 \) unknowns: the \( n \) potential slip rates in each grain (\( \dot{\gamma}_s^I \) and \( \dot{\gamma}_s^H \)) and the 2 shear relaxations \( \dot{\gamma}_{13}^L \) and \( \dot{\gamma}_{23}^L \). By treating the relaxations as “pseudo slip-systems” having a critical resolved shear stress equal to zero, the constrained minimisation can still be solved using linear programming (Van Houtte, 1988). It has been demonstrated (Van Houtte et al, 1999) that the resulting stress state is such that \( \sigma_{13}^I = \sigma_{13}^H \) and \( \sigma_{23}^I = \sigma_{23}^H \), thus improving stress equilibrium relative to the FC Taylor solution. This can be foreseen intuitively from the observation of Fig. 3.1: since grain boundary sliding is forbidden, a grain may shear only if it “drags” its neighbour accordingly. Due to the difference in lattice orientation, a relaxation \( \dot{\gamma}_{13}^L \) (or \( \dot{\gamma}_{23}^L \)) that reduces \( \dot{W}_I \) (and would be predicted by the RC pancake model), but leads to an increase of \( \dot{W}_H \), will not be predicted by the LAMEL model. By minimising the energy dissipated in total, \( \dot{W}_{TOT} = \dot{W}_I + \dot{W}_H \), a compromise relaxation is predicted that corresponds to stress equilibrium.

To further illustrate how the LAMEL model yields intermediate results between FC Taylor and RC pancake, one may compare the values of the Taylor factor and of the relaxed shear strain (absolute values) averaged over a random texture. This is done in Table 1 and 2 for either bcc or fcc slip.

<table>
<thead>
<tr>
<th>Table 1 Predicted Taylor factor and relaxed shears (bcc slip)</th>
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<tbody>
<tr>
<td><strong>M-factor</strong></td>
</tr>
<tr>
<td>Avg (</td>
</tr>
<tr>
<td>Avg (</td>
</tr>
</tbody>
</table>

\(^{(1)}\) 1=RD ; 2=TD ; 3=ND.
Table 2 Predicted Taylor factor and relaxed shears (fcc slip)

<table>
<thead>
<tr>
<th></th>
<th>FC Taylor</th>
<th>LAMEL</th>
<th>RC pancake</th>
</tr>
</thead>
<tbody>
<tr>
<td>M-factor</td>
<td>2.87</td>
<td>2.68</td>
<td>2.50</td>
</tr>
<tr>
<td>Avg</td>
<td>d</td>
<td>_13/</td>
<td>d</td>
</tr>
<tr>
<td>Avg</td>
<td>d</td>
<td>_23/</td>
<td>d</td>
</tr>
</tbody>
</table>

With respect to the FC Taylor theory, the relaxations \( \gamma_{13}^L \) and \( \gamma_{23}^L \) constitute two degrees of freedom. This means that a minimum of 8 slip systems, instead of 10, must be activated on the whole, for the two grains. Depending on the interacting lattice orientations, it is possible that each grain activates 4 slip systems, or that one grain activates 5 systems and the other only 3. The latter situation is illustrated in Fig. 3.2 showing the two yield loci. In this general example, the solution corresponds to a corner stress in grain I (5 systems activated) but a 2-dimensional facet in grain II (3 systems activated). Only this combination provides equal stress and opposite strains, at the same time, while fulfilling the normality rule. Furthermore, as only one corner solution is left, the number of equally stressed slip systems is reduced and the Taylor ambiguity is less important than under FC Taylor (Chapter 1).

In all Taylor-type models, the lattice spins are derived from the slip rates computed in the energy minimisation (Chapter 1). Applying this to the LAMEL model, it is clear that the lattice rotation of a grain depends on the orientation of the interacting neighbour. Two grains having the same initial orientation but a different neighbour thus rotate towards different end-orientations. Note also that, before the simulation starts, the two grains are selected at random out of a
Chapter 3  Theories about grain interactions and subdivision

set of orientations representing the initial global texture. They thus have a random misorientation. However, due to the interaction of the two grains, their misorientation may have a special character at the end of the simulation. The build-up of such “microtexture” will be investigated in Chapter 4.

1.2 Other models overlooking in-grain heterogeneities

In the “modified Sachs model” by Pedersen and Leffers (1987), grain interactions are considered in a stochastic manner by introducing random stress perturbations relative to the Taylor solution. This model can thus not really be seen as a “N-site” model although two grains with the same initial orientation follow distinct deformation paths.

In their “neighbourhood compliance” model, Sarma and Dawson (1996b) consider clusters of ~10..1000 grains at a time. The topology of the grain arrangement is not accounted for, but two initially identical grains deform distinctly if they belong to different clusters. This “neighbourhood compliance” model is based on the model by Chastel and Dawson (1993) where the “cluster” consisted of the whole polycrystal (Chapter 1). Sarma and Dawson (1996b) make supplementary assumptions, stating that the symmetric part of $l_{ij}$ is proportional to the “relative compliance” of a grain with respect to its neighbours. The skew-symmetric part of $l_{ij}$ is then approximated by imposing that symmetric and skew parts of $l_{ij}$ deviate in the same way from the macroscopic values.

The GIA model developed by P. Wagner at RWTH (Aachen, Germany) and used by Raabe (1995a,b) resembles the LAMEL model as it allows grains to shear superimposed to the macroscopic plane strain compression. Here also, shears are partly constrained contrarily to what is assumed in RC Taylor models. Grains shear proportionally to their “shear capacity”, i.e. to the gain of energy achieved by relaxing the shear divided by the shear itself (~ to the slope of the energy decrease associated with the relaxation). There is also a normalisation by the highest shear capacity present in the texture.

The most elaborated models belonging to this class are certainly the N-site self-consistent models (Canova et al, 1992; Lebensohn and Canova, 1997). These models have the same architecture as the 1-site self-consistent models of Chapter 1, but here the inclusion is a cluster of interacting grains instead of just 1 grain. They are also used for studying interactions in multiphase materials.
Chapter 3  Theories about grain interactions and subdivision

2  Grain-scale FE models

The finite element (FE) method can be used as a “computational microscope” providing a 3-dimensional map of the lattice orientation, the strain and the stress in the bulk of a plastically deforming polycrystal. The rule applied to partition deformation among the constituting crystallites is much more realistic than in any of the classical plasticity theories. Indeed, in FE modelling, the continuity of displacement and the equilibrium of stress are ensured throughout the crystallite aggregate. For this, all components of the stress and the velocity gradient tensors must have the opportunity to vary within individual grains. From the point of view of texture modelling, the FE element method predicts the development of in-grain orientation gradients as well as the effect of a grain’s direct neighbourhood on the evolution of its mean orientation.

In practice, the local lattice orientation (as well as CRSS describing the hardening history) is viewed as a state variable that varies from point to point over the FE mesh representing the polycrystalline aggregate. Single crystal plasticity equations serve to derive the flow properties at several points (termed “integration points”) within each grain. Rate-dependent formulations have often been favoured (e.g. Becker, 1991; Kalidindi et al, 1992) with the exception of Knockaert et al (2000). The FE method requires extensive computational power because the plasticity equations are integrated at once for the whole aggregate, and because the deformation field can be determined only by solving the overall equilibrium equations iteratively.

In order to fulfil stress equilibrium and strain compatibility at grain boundaries, each grain must be represented by at least one cubic element with 8 nodes. In this most simple case, the velocity gradient, the stress and the slip rates are predicted to vary linearly in whichever direction across individual grains. This means that the lattice orientation is also assumed to vary constantly from one grain edge to another. More complex in-grain heterogeneities can be modelled by utilising several such elements per grain (e.g. Becker, 1991) or by constructing grains of rhombic dodecahedral shape (12-sided space-filling polyhedra) each made of 48 tetrahedral elements with 10 nodes as Mika and Dawson (1998) did. Obviously, the computational work involved in a simulation increases with the number and the type of elements. Dawson and his collaborators rely therefore on parallel computing on powerful workstations. They furthermore make use of a “hybrid FE formulation” that overcomes some
convergence problem related with the discontinuity of the material law due to the lattice misorientation at grain boundaries (Beaudoin et al, 1995).

Grain-scale FE models are generally used in two types of investigations. When each grain is represented e.g. by a single cubic element, the topology of the real polycrystalline aggregate can be reproduced only in a very crude way. In this case, the aim of the simulation is not to analyse how deformation is distributed among this particular grain arrangement, but rather to predict the macroscopic constitutive law or the evolution of the global texture (Kalidindi et al, 1992; Beaudoin et al, 1995). Such results constitute a valuable reference for developing models that are faster and less elaborated, such as the LAMEL model. In the second type of grain-scale FE simulations, the purpose is to reproduce as closely as possible the deformation field observed experimentally over a multicrystal counting few coarse grains (Becker, 1991; Becker and Panchanadeeswaran, 1995; Delaire et al, 2000; Bhattacharyya, in press). In order to obtain an accurate map of in-grain heterogeneities, many elements are used to represent each grain (Fig. 3.3a). Nevertheless, such FE simulations have in general had a limited success in predicting the shape-change of the grains, their lattice rotation and their subdivision. This is most probably due to the fact that FE models consider just one origin of in-grain heterogeneity: the interaction with surrounding grains. In the next section, we will see that there are other driving forces to the formation of in-grain heterogeneities.

Fig. 3.3 Difference between a) “grain-scale” and b) “full-scale” FE simulations. a) Reproduction of the microstructure in a coarse-grained tension-test specimen. b) Cup-drawing simulation wherein each integration point represents a polycrystal (Winters, 1996).
Finally, it must be stressed that it is still unfeasible to apply “grain scale” FE codes in full-scale simulations of deformation processes (Fig. 3.3b), the main reason being that computers are not powerful enough. In full-scale FE simulations, each integration point has a polycrystalline constitutive law. Usually, it is assumed that this polycrystal undergoes a uniform deformation (Taylor assumption). The texture of the polycrystal is thus the state variable from which the local plastic anisotropy is predicted.

3 Simulating grain subdivision in the absence of interactions with the surrounding grains

The theories to be presented now explain the development of in-grain heterogeneities without having to account for interactions of the grain with its surrounding. The first two theories focus on the amplification of an existing heterogeneity. Then, we address the creation of this initial in-grain heterogeneity.

3.1 In-grain orientation gradients due to divergent rotations in Euler space

Dillamore and Katoh (1974) proposed a model that supports their experimental observation of long-range lattice curvatures within grains of fcc polycrystals. Their idea is that the orientation space can be subdivided into domains, each rotating towards a different texture component (under PSC). If the initial orientation of a grain lies precisely at the border between two such domains, two regions of the grain may rotate towards end-orientations that are very remote of one another. According to the authors, the misoriented regions would be separated by a “transition band” accommodating a continuous lattice curvature. It is noteworthy that such heterogeneity may arise even under homogeneous strain (i.e. no grain interaction). However, the model does not predict when an initial misorientation arises between the two subgrain regions so that they come to lie in different domains of Euler space.

Due to its high symmetry, the cube \( \{001\}<100> \) orientation lies at the border of several orientation domains. Therefore, many transition bands have a \( \{001\}<100> \) oriented nuclei. According to Dillamore and Katoh (1974), the high lattice curvature promotes subgrain growth upon annealing, which explains the predominance of the cube component in recrystallisation textures.
3.2 Splitting due to a deformation heterogeneity that “cancels out” at the grain level

An idea that is used by several researchers (Leffers, 1991; Lee and Duggan, 1993; Butler and McDowell, 1998) is that grains split into fragments having heterogeneous deformations and achieving the macroscopically imposed deformation only collectively, at the grain scale. Similarly to the RC theories and the LAMEL model, the driving force for the local strain heterogeneities is a reduction, with respect to FC Taylor, of the internally dissipated energy. A supplementary resemblance with the LAMEL and RC models is the assumption that less than 5 slip systems need to be activated within each subgrain. (For the LAMEL and RC models, it is within each grain.)

Both Leffers (1991) and Lee and Duggan (1993) assume that the fragments undergo simple shear deformations superimposed on the macroscopic shape change. Their models are actually very similar to the LAMEL model (Chapter 1) except that they consider interactions between subgrains instead of interactions between adjacent grains. Leffers (1991) applied this idea to low-strain subdivision into cell blocks with relaxation-shears occurring in a plane at 45° to the rolling plane; whereas Lee and Duggan (1993) considered high-strain deformation banding with shears parallel to the plane RD-ND. Lee and Duggan (1993) thus account for a type of deformation banding that is not so frequent: usually, deformation bands are observed parallel to the rolling plane. The two models are illustrated in Fig. 3.4.

![Fig. 3.4 Illustration of the subdivision models proposed by a) Leffers (1991), and b) Lee and Duggan (1993).](image)
It must be noted that none of these models can predict the thickness of the banded fragments. Furthermore, as stressed by Leffers (1995), these models do not explain how subdivision is triggered. Indeed, at the onset of subdivision, the two fragment families have exactly the same initial orientation. In that case, whatever the value of the opposite shears, the total dissipated energy can only be equal to its value under FC Taylor (no splitting). Indeed, due to the assumed linearity of the plastic work, any reduction obtained by shearing one fragment family would be exactly compensated by the increase of energy necessary for shearing the other fragment family in the opposite sense. On the other hand, a lower number of slip systems needs to be activated when splitting occurs so that the probability to create dislocation jogs is reduced (Leffers, 2001). In order to apply the latter idea in predictive simulations, it is necessary to incorporate some ideas from dislocation patterning theories (section 3.4).

### 3.3 The Taylor ambiguity, source of in-grain heterogeneity

We have seen in Chapter 1 that many deformation modes can be achieved by several slip-system combinations. These combinations are equally probable as they imply (i) the activation of slip systems that are identically stressed, and (ii) an equal dissipation of energy. This was called the “Taylor ambiguity”. It is thus conceivable that a uniformly deforming grain be split into volumes that activate different such combinations of slip systems. Initially, the stress, the velocity gradient and the internally dissipated energy would be the same in all subdivided volumes. Only the lattice spin would be different and would give rise to misorientations between adjacent volumes. Such misorientations could, at least in some grains, lead to an increased heterogeneity of slip and be subsequently associated with heterogeneity of stress and dissipated energy.

The Taylor ambiguity was recognised by Chin (1969), as one origin of deformation banding.

### 3.4 Dislocation patterning, source of in-grain heterogeneity

Many of the microstructural features described in Chapter 2 cannot be explained by “continuum theories” in which dislocations are viewed only as the unit carrier of plastic strain. Experimentally, one finds that the dislocation density varies significantly over the crystal lattice. Dislocations tend to cluster and to fragment the grain into volumes that are almost free of dislocations delineated by “walls” with a high dislocation content. The characteristic
dislocation patterns that are formed are observed at a scale much lower than the scale of the orientation and/or strain gradients expected from grain interactions. Furthermore, the same patterns are encountered in single crystal experiments in which there are no neighbouring grains. In order to simulate this fragmentation, one has no alternative but to acknowledge that dislocations interact with one another and that the length-scale of subdivision is related to the mean free path of a mobile dislocation.

The basics of dislocation patterning theories can be summarised as follows:

1° Dislocations are irregularities of the crystal lattice and have therefore an associated long-range stress field.

2° Dislocations tend to arrange themselves into configurations that permit significant screening of the associated stress fields. Some examples are dipolar walls, “Taylor lattices” and 3-dimensional cellular arrays. The energy that can be spared by adopting such configurations has been estimated (Hansen and Kuhlmann-Wilsdorf, 1986).

3° When a dislocation wall is formed, it not only creates an obstacle to the motion of other dislocations (as evidenced by the observation of dislocation pile-ups), it also gives rise to a misorientation of the lattice on either side of the wall.

4° If dislocation screening is complete (i.e. if no long-range stress is left), there is a univocal relationship, termed “Franck’s rule”, between (i) the angle and axis of lattice misorientation at a wall, (ii) the macroscopic directionality of the wall, and (iii) the dislocation content of the wall (Kuhlmann-Wilsdorf, 1962). The misorientation increases during monotonic deformation as the wall captures more dislocations with similar Burgers vectors. In practice, Franck’s rule has been applied to estimate the dislocation content of a wall from its experimentally measured misorientation and tilt (e.g. Wert et al, 1995).

Most researchers agree that the observed dislocation structures have a lower energy than if dislocations were randomly distributed over the lattice. However, it is still an open question whether the dislocation patterns may be considered as free of long-range stresses, i.e. whether point 4° applies. It is also not evident that dislocation patterning is governed predominantly by the minimisation of the energy of dislocation interaction.
For our present purpose, it is sufficient to recognise that dislocation interaction has the potential to accentuate the heterogeneity of deformation by fragmenting the grain into small volumes having finite lattice misorientations. Variations in the strain and stress fields, thereby, appear on top of the gradients expected from grain interactions.

Finally, one should note that dislocation slip and dislocation patterning are interrelated. The dislocation pattern that is created depends on the local deformation and on the slip activity, i.e. on the type and the amount of dislocations that are potentially immobilised. A proof is that extended planar dislocation walls of moderate-strain rolling microstructures (DDWs and MBs) are created parallel to the most stressed slip system (see Chapter 2). Reciprocally, the observation of pile-ups proves that immobilised dislocation patterns constitute obstacles to mobile dislocations. Dislocation walls thus augment the slip resistance along the intersected crystallographic planes (e.g. Peeters et al, 2001; Seefeldt et al, in press). As the immobilised dislocation structure has a strong directionality, it hardens each slip system to a different extent. Consequently, some slip system may harden sufficiently to be replaced by others that would have remained inactive in the absence of a dislocation substructure because they are less favourably oriented with regard to the macroscopic stress (Chapter 1). Note also that the Taylor ambiguity is solved when each slip system has a different slip resistance, i.e. a different $\tau'_c$. The anisotropic slip resistance is thus likely to affect both the local stress and strain, and the global evolution of texture.

4 Conclusion

This chapter has presented an overview of various tools permitting the simulation of grain interactions and of the build-up of intra-granular heterogeneities. Due to the great complexity of the micromechanics involved in the creation of in-grain heterogeneities, none of the existing models allows simulating all the features observed in Chapter 2. The fragmentation of the grain at the finest scale can be predicted only if one takes account of dislocation patterning. However, there is still much disagreement on how to implement this in predictive simulations. Therefore, these aspects are excluded from the second part of the thesis.
Chapter 3  Theories about grain interactions and subdivision

The simulations and the experimental observations carried out in this work have as main objective to determine whether the LAMEL model and/or a FE model provide a reliable estimate of the effect of grain interactions on the average deformation of individual grains and on the gradients developing within them. As the FE simulations make use of a single 8-noded element to represent each grain, both models rely on a crude representation of the microstructure. Such models are however chosen because their application in macroscopic simulation does not require too much increase of the available computational power, and may thus be expected for the near future.

The performances of the two models simulating grain interactions will be evaluated in two ways:

- In Chapter 4, we will check whether the evolution of the global texture is better simulated when two grains having the same orientation but a different neighbourhood are considered not to undergo the same deformation.

- In Chapter 6, we will measure the orientation spread predicted to develop within a grain due to the interaction with its neighbours. We will see that the LAMEL model as well as the FE model can serve for such predictions, and that their assumptions are different.

- The intra-granular orientation gradients predicted in Chapter 6 will be compared to experimental measurements presented in Chapter 5. For this, a new analytical method will be proposed, which allows a characterisation and a quantification of grain subdivision from local orientation data recorded by OIM.
CHAPTER 4: PERFORMANCE OF VARIOUS TEXTURE PREDICTION MODELS – IMPROVEMENT OF THE LAMEL MODEL

In this chapter, we evaluate whether predictions of rolling textures are improved when using plasticity models that account for grain interactions. First, some short comments are made about the textures developing in cold rolled metals, and a set of tools is proposed for an accurate quantitative texture characterisation. Second, the four plasticity models selected for the simulations are presented as well as the method used for solving Taylor ambiguity. Texture simulation results are then presented, starting with a description of the reference experimental textures. It turns out that predictions are less accurate under fcc slip than under bcc slip. Therefore, an elaborated version of the LAMEL model is proposed and it is shown that the new model yields almost as accurate predictions as FE models, whereas much less computing time is required. Some comments are finally made about the development of microtexture, i.e. the final misorientation between two interacting grains, and about the effect of the choice made for solving the Taylor ambiguity.

1 Characterisation of rolling textures in cubic metals

1.1 Bcc rolling textures

In the next section, several plasticity models will be used to simulate texture development during cold rolling of steel plates. These plates are ferritic when cold rolled although they were hot rolled in the austenitic range. The input texture for our simulations is the so-called “hot band” texture resulting from the fcc \(\rightarrow\) bcc phase transformation occurring after hot rolling (Ray et al, 1994). This transformation texture is weak if hot rolling is performed at very high temperatures so that recrystallisation occurs. Otherwise, the hot band texture is
somewhat stronger and it resembles a cold rolling texture (as illustrated in section 3). Whatever the hot band texture, two crystallographic fibres develop upon cold rolling: the $\alpha$-fibre containing orientations with a $<110>$ axis parallel to RD, and the $\gamma$-fibre gathering orientations with a $<111>$ axis parallel to ND (1). The two fibres thus intercept one another at the $E \{111\}<110>$ component and they are both visible in the $\varphi_2=45^\circ$ section of the Euler space (Fig. 4.1). Other important components of bcc rolling textures, $F \{111\}<112>$, $I \{112\}<110>$ and $H \{001\}<110>$, are also highlighted in Fig. 4.1.

Fig. 4.1 Representation in 3 dimensions of the four ODF sections used to reveal the typical fibres and individual components in bcc rolling textures.

A peculiarity of the $\gamma$-fibre is that it is composed of three symmetrically equivalent segments ($E-F$, $F-E$ and $E-F$ in Fig. 4.1). In describing the fibre, it is sufficient to consider one segment, for example from $\varphi_1=60^\circ$ to $\varphi_1=90^\circ$. Note also that the theoretical definition of the $\gamma$-fibre ($\{111\}//ND$) is only an approximation of reality. In practical cases, the $\gamma$-fibre can be shifted of up to 10-15 degrees in Euler space. In order to reveal these shifts, ODFs will here be represented, not only by their $\varphi_2=45^\circ$ section, but also by the sections $\varphi_1=60^\circ$, $75^\circ$ and $90^\circ$ that are perpendicular to the $\gamma$-fibre. The $\alpha$-fibre, on the other hand, lies along a symmetry axis of the Euler space, which ensures a more constant

(1) The letters $\alpha$ and $\gamma$ have, here, nothing to do with the austenite and ferrite phases.
position. Finally we should mention that the $\alpha$-fibre tends to disappear during the annealing treatment that follows cold rolling whereas the $\gamma$-fibre comes closer to its theoretical position. This gives rise, by chance, to the best deep drawing properties that a texture can offer.

It has been shown\textsuperscript{(1)} that, by focusing on the crystallographic fibres, rolling and recrystallisation textures in steel can be characterised with far less parameters than the harmonic series expansion coefficients. This parameter model for texture description was employed to estimate how the planar anisotropy of a plate is affected by small perturbations of the plate texture. For this, the $\Gamma$-value, i.e. the ratio of the transverse and normal strain rates during a traction test on a plate, was predicted by applying the FC Taylor model (Schouwenaers et al., 1994). The sensitivity study showed that small variations in the position of the $\gamma$-fibre or in the ODF intensity distribution along the fibres could have dramatic effects on the mechanical anisotropy of the plate. From this study, it was also concluded that it is insufficient to describe a fibre only by its position in Euler space and by the ODF intensity distribution along the skeleton line (i.e. line of maximum intensity / “axis” of the fibre). For a more accurate characterisation, one must also estimate the fibre “thickness”, i.e. how fast the ODF intensity decreases from the fibre centre to remote orientations in a section perpendicular to the fibre axis.

In view of this, we have developed a new procedure that locates fibres more accurately in Euler space, and that also measures the fibre thickness. Locating a fibre in Euler space amounts to determining the maximum ODF intensity in perpendicular sections lying at regular intervals along the fibre. As harmonic series are too elaborated for a mathematical derivation, the maximum intensity (fibre centre) is traditionally identified in a set of discrete ODF values over a $5^\circ$ grid representing the fibre section (Fig. 4.2). In the new method, however, a better estimation of the real maximum is obtained by considering that the series expansion can be locally approximated by a $4$th order polynomial. One such polynomial is given in Eq. 4.1, where the variables $x$ and $y$ define locations in the ODF section and would correspond to $\phi$ and $\phi_2$ in the case of a $\gamma$-fibre.

\begin{equation}
\sum_{h=0,4,4} \sum_{k=0,4} a_{hk} x^h y^k
\end{equation}

\textsuperscript{(1)} That study is not included in the thesis. Complementary information can be found elsewhere (Delannay et al, 1999, 2000).
The coefficients $a_{hk}$ of the polynomial are determined by fitting the ODF values over a $20^\circ \times 20^\circ$ grid around the discrete maximum in the section (Fig. 4.2). The location of the fibre centre $(x_c, y_c)$ corresponds to the maximum value of the polynomial, and it is derived using a non-linear optimisation routine.

Supplementary to the three parameters $x_c, y_c$ and $f(x_c, y_c)$, the ODF section is also characterised by the “fibre thickness”. In practice, we compute the integral of the ODF intensity (numerically) over a $30^\circ \times 30^\circ$ grid around the fibre centre. This integral can be seen as the product of the “fibre thickness” and the maximal intensity $f(x_c, y_c)$. The integral is actually a good estimate of the volume fraction of crystallites oriented close to the centre of the fibre section.

The suggested procedure yields an accurate description of the $\gamma$-fibre, and it can easily be adapted to characterise the $\alpha$-fibre (as well as the fibres encountered in fcc metals). In the following, the performance of the various polycrystal plasticity models will be judged on their ability to predict the location and the integral/intensity distributions along crystallographic fibres, for different starting textures. Predicted r-value profiles will also be compared, as we know that they are sensitive to texture and are also important for industry.

A final tool for estimating the quality of a texture prediction is the “texture index” (T.I.) (Bunge, 1982) of the difference between the predicted ODF, $f_{\text{sim}}(g)$, and the experimental ODF, $f_{\text{exp}}(g)$. This texture index gives an overall appreciation of the texture reproduction, combining information about the position and strength of the fibres in just one parameter. It can efficiently be computed from the harmonic series coefficients:

$$T.I. = \frac{1}{2} \int \left[ f_{\text{sim}}(g) - f_{\text{exp}}(g) \right]^2 dg = \sum_{l=1}^{L_{\text{MAX}}} \frac{1}{1 + 2l} \sum_{\mu \nu} \left( C_{\mu \nu, \text{sim}}^{l} - C_{\mu \nu, \exp}^{l} \right)^2$$ (4.2)
1.2 Fcc rolling textures

Only aluminium textures are considered here. This is because of the industrial relevance of aluminium and because the texture development is relatively similar in other fcc metals where a high stacking-fault energy (SFE) prevents twinning. Cold rolling simulations in aluminium take on input a “hot band” texture that corresponds to the recrystallised plate at the exit of the hot rolling mills and that has as major component the cube {001}<100> orientation. During cold rolling of such fcc metal, two crystallographic fibres arise, which were described by Hirsch and Lücke (1988) as the $\alpha$-fibre containing orientations with $<110>$/ND and extending from Goss {110}<001> to brass {110<112>, and the $\beta$-fibre starting at brass, running through S {123}<634> before it reaches copper {112}<111> (see Fig. 4.3). The $\beta$-fibre contains the most stable components of the rolling texture, but the ODF intensity distribution along the fibre depends on the material: low-SFE metals yield a strong brass component whereas high-SFE metals favour rotations to the copper and S orientations. Note that the $\beta$-fibre lies close to the $<111>$/RD fibre that would be produced if the material were deformed by uniaxial tension along RD.

Fig. 4.3 Representation of some typical fibres and single components in fcc rolling textures. (C= cube, RDC= RD-rotated cube, TDC= TD-rotated cube, G= Goss, B= Brass and Cu= copper).
After moderate rolling reductions of aluminium plates, remnants of the original cube texture may still be observed in the ODF. It is then necessary to also describe ODF intensities measured at cube as well as rotated cube orientations. We will, for this purpose, distinguish between the RD-rotated cube \{025\}<100> and TD-rotated cube \{205\}<502> components that are generated by rotating the \{001\}<100> component of \sim22° around RD and TD, respectively. We will also define a “cube-fibre” that extends from RD-rotated cube, via cube, to TD-rotated cube (also indicated in Fig. 4.3).

Three ODF sections suffice to show all important components of fcc rolling textures. These sections are presented in Fig. 4.3. The $\phi_2=90°$ section shows the $\alpha$- and the cube-fibre. It is also perpendicular to the $\beta$-fibre, which is also true for the $\phi_2=65°$ and $\phi_2=45°$ sections revealing the strength and exact location of the $S$ and copper components.

In the aluminium textures considered here, the cube-fibre turns out to be more interesting than the $\alpha$-fibre. Therefore, the ODF will be characterised by focusing only on the cube-fibre and the $\beta$-fibre. Moderate as well as high rolling strains will be considered, so as to relate texture evolution to the subdivision mechanisms presented in Chapter 2 and further studied in Chapter 5. In cases where the $\beta$-fibre is sufficiently clearly formed, its skeleton line will be located by applying the procedure presented in the previous section. The various texture prediction models will be evaluated by comparing profiles of ODF-intensity integrals calculated perpendicular to the two fibres.

2 Plasticity models to be compared

Four plasticity models have been selected for the comparative study. Among them, the “full constraints” (FC) Taylor model and the “relaxed constraints pancake” (RCP) model represent the classical theories of polycrystal plasticity that were reviewed in Chapter 1. Two more elaborated models that account for interactions of each grain with a specific neighbourhood are also taken into consideration: the LAMEL model and a FE model.

The same initial grain orientations are used for all simulations. These orientations are generated by discretising, with the algorithm proposed by Toth and Van Houtte (1992), the texture measured on the undeformed plate. The simulated ODFs are reconstructed by superposing gaussian distributions with a half-scatter width of 7° on the final grain orientations as is traditionally done.
2.1 Some comments about the FE simulations

The FE model consists of the implementation by Kalidindi et al (1992) of single-crystal plasticity as a “user defined material law” in the ABAQUS code. The simulations are performed on a mesh containing 1200 cubic elements with 8 integration points, and each element represents a grain (as already suggested in Chapter 3). The initial mesh as well as an example of a 70% compressed mesh are shown in Fig. 4.4.

In such simulation, the lattice rotation that a given grain undergoes depends significantly on its position in the mesh and on the orientation of its direct neighbours (this is investigated in detail in Chapter 6). However, we have checked that the topological arrangement of the grains has negligible effect on the predicted overall texture, as long as the lattice orientations are randomly distributed over the mesh.

The boundary conditions on the mesh are such that all outer surfaces remain planar, except for those normal to RD.
2.2 Solution of the Taylor ambiguity

Except for the FE simulations, all selected models rely on a rate-independent formulation of single crystal plasticity. This means that the texture predictions depend on the choice made for solving the Taylor ambiguity (Chapter 1). A new procedure has been developed that computes all energetically equivalent sets of slip rates achieving the local strain and that allows making whichever selection among them. It proceeds as follows.

- As already discussed in Chapter 1, a first set of valid slip rates can be found using linear programming (Van Houtte, 1988). This also determines the stress tensor and the Taylor factor that are common to all energetically equivalent solutions.

- Knowing the stress tensor, one may calculate resolved shear stress on all potential slip systems \( \tau_s = M_{ij}^s \sigma_{ij} \), and assess whether the number of critically stressed slip systems is larger than what is strictly necessary. Five slip systems are necessary under full constraints (“corner stress”), whereas three or four slip systems suffice under relaxed constraints (stress perpendicular to a rib of the yield surface).

- Let us suppose that \( n_{active} \) slip systems have a resolved shear stress \( \tau_s \) equal to the critical value \( \tau_s^c = 1.0 \), whereas the local strain could already be achieved by activating a combination of only \( n_{needed} \) out of the \( n_{active} \) slip systems. This does not mean that all such combinations yield a valid slip-rate solution. Indeed, some combinations may include slip systems that are not (geometrically) independent of one another and that can thus not fulfil the prescribed strain. Furthermore, a combination is also invalid if negative slip rates are needed to produce the strain. The method used to check if a given slip-system combination leads to a valid solution relies on linear programming. This time, not all \( \tau_s^c \) are set to 1.0: only the \( n_{needed} \) belonging to the combination are set to 1.0, the \((n_{active} - n_{needed})\) others are artificially set to 10.0. Since the linear programming routine minimises the deformation energy, it activates preferentially the slip systems with the lower CRSS. However, if no valid solution can be found then other systems are activated and the dissipated energy is raised (due to the higher CRSS). The latter cases are thus easily excluded from the analysis.

If \( N_{valid} \) valid solutions are found (each involving a distinct set of \( n_{needed} \) out of the \( n_{active} \) slip systems), any positive linear combination of these \( N_{valid} \) valid
solutions also constitutes a valid solution. We thus have to define a criterion dictating the weights to be assigned to each of the $N_{\text{valid}}$ valid solutions. The criterion that is applied in this work states that slip should be distributed as much as possible on all critically stressed slip systems. It turns out that this choice permits a significant improvement of FC Taylor predictions of fcc rolling textures compared to other criteria (see section 4). The weights $w_k$ assigned to the valid solutions ($k=1..N_{\text{valid}}$) are thus determined by minimising

$$\sum_{s=1}^{N_s} \left( \sum_{k=1}^{N_{\text{valid}}} w_k \tilde{Y}_{sk} \right)^2.$$  

(4.3)

Previously, the slip rates were determined by rounding off the yield locus (Van Houtte and Rabet, 1997). This method was computationally fast, but convergence problems occurred when solutions were to be found along ribs or facets of the yield surface (i.e. when applying the pancake RC model or the LAMEL model). The new method overcomes this, and is thus also advantageous when relying on RC models even though the Taylor ambiguity effect is marginal in those cases. Table 1 shows the computing times required for simulating rolling up to 70% thickness reduction. All simulations were performed on a Pentium II (233MHz-64MbRAM) except for FE simulations that are carried out on a Sun Ultra 2 (300MHz-256MbRAM) workstation. It is noteworthy that $N$-site models (LAMEL/FEM) are applied to a larger number of discrete orientations. This ensures that each orientation interacts with a representative sampling of its potential neighbours in the real material.

<table>
<thead>
<tr>
<th>Table 1 Number of grains and time required by the simulations.</th>
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<tbody>
<tr>
<td><strong>Number of grains used in a simulation</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Taylor FC</td>
</tr>
<tr>
<td>Taylor RC (Pancake)</td>
</tr>
<tr>
<td>LAMEL</td>
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<tr>
<td>Finite Element Model</td>
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</tbody>
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(1) This means 3000 lamellas, each containing 2 grains. (2) Thus, $1200 \times 8 = 9600$ integration points that are able to develop distinct orientations.
The larger computing time required by FC Taylor compared to RC pancake is due to a greater ambiguity in the solutions. Also, the 12 slip systems under fcc lead to more ambiguity (proportionally) than the 24 systems under bcc. Finally, it must be stressed that although our FE simulations are oversimplistic compared to what e.g. Mika and Dawson (1996) did (i.e. 480 integration points to represent each grain), they already require much more computing time than all other prediction models.

3 Texture predictions in steel

In order to test the prediction models under bcc slip conditions, two industrial steel plates were selected. The first is an ultra low carbon (ULC) steel having an almost random “hot band” texture (max ODF intensity: 2.9). The second is an interstitial free (IF) steel showing a rolling-type texture already before cold rolling started (max: 12.4). Both plates were cold rolled to a thickness reduction of 70% (equivalent strain of 1.2). The ODFs representing the initial and the final texture were derived from X-ray texture measurements performed in MTM. The ODFs representing the input textures are shown in Fig. 4.5 whereas the ODFs measured after cold rolling are given together with the simulation results to allow a direct comparison.

Fig. 4.5 ODFs representing the experimental bcc textures prior to cold rolling. Contours: 1 / 3 / 7.5.

The two materials develop rolling textures that differ mostly by the location of the γ-fibre and by the strength of the α-fibre, as illustrated in Fig. 4.6. In the
IF steel, the major effect of cold rolling is to increase the $\alpha$-fibre strength (Fig. 4.6b) whereas the $\gamma$-fibre maintains an almost constant strength (Fig. 4.6c), being only shifted in Euler space (Fig. 4.6a). Conversely, the $\gamma$-fibre strengthens significantly more than the $\alpha$-fibre in the ULC steel.

The ODFs shown in Fig. 4.7a-b represent the textures predicted to arise in the two steels after 70% cold rolling. A thorough texture comparison that focuses on the predicted skeleton lines is given in Fig. 4.8.

(1) The $\gamma$-fibre localisation is impeded in the undeformed ULC steel that has a too weak texture. The ODF-integrals are computed at the same location as in the 70% c.r. plate.
Fig. 4.7a Comparison of the experimental ODF in the 70% C.R. ULC-steel to the ODFs predicted by various texture models.

Contours: 1 / 3 / 7 / 15 / 25.
**ULC-steel C.R. 70%**

<table>
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Fig. 4.7b Comparison of the experimental ODF in the 70% C.R. ULC-steel to the ODFs predicted by various texture models. Contours: 1 / 3 / 7 / 15.
Chapter 4  Performances of various texture models

Fig. 4.8a Accurate localisation of the $\gamma$-fibre (IF-steel).

Fig. 4.8b ODF intensities along $\alpha$ and $\gamma$ (IF-steel).

Fig. 4.8c ODF-Integrals in sections perpendicular to $\alpha$ and $\gamma$ (IF-steel).
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Fig. 4.8d Accurate localisation of the $\gamma$-fibre (ULC-steel).

Fig. 4.8e ODF intensities along $\alpha$ and $\gamma$ (ULC-steel).

Fig. 4.8f ODF-Integrals in sections perpendicular to $\alpha$ and $\gamma$ (ULC-steel).
After analysis of the skeleton lines in Fig. 4.8a-f, it is clear that the LAMEL and FE model accounting for grain interactions yield predictions that are much closer to the experimental textures than the classical plasticity theories.

- Along the $\gamma$-fibre, the ODF-intensity as well as its integral in sections perpendicular to the fibre are perfectly reproduced by the LAMEL and FE model. This is not at all the case for the Taylor FC and RC models that predict, respectively, too high and too low intensities at $F\{111\}<112>$. The position of the fibre is better predicted for the IF steel than for the ULC steel in which the $\gamma$-fibre is almost perfectly aligned with the “ideal fibre” $\{111\}$//ND.

- The strength of the $\alpha$-fibre is also better estimated by the two models that take account of grain interactions. The prediction is however not as good as for the $\gamma$-fibre, especially, close to the $H\{001\}<110>$ component at the “top” of the fibre.

Even though the LAMEL and FE model predictions do not match exactly the experimental textures, it is remarkable that they yield a quantitative prediction of (at least) the strength of the $\gamma$-fibre, starting with two very different textures. This constitutes a great improvement compared to the classical FC and RC theories, which is also revealed by computing the texture index of the difference between the predicted and the experimental textures (Table 2).

<table>
<thead>
<tr>
<th></th>
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<th>RCP</th>
<th>LAMEL</th>
<th>FEM</th>
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<td>ULC 70%</td>
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<td>1.8</td>
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<td>4.6</td>
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(1) All texture indexes are computed with LMAX= 32.

Finally, it is interesting to compare the $r$-value profiles that correspond to the predicted and the experimental textures (Fig. 4.9). One observes an excellent reproduction of the $r$-value profile in the IF steel. Apparently, such profiles are influenced more by the $\gamma$-fibre strength and position (“harder” texture components) than by the $\alpha$-fibre strength (“softer” texture components).
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Fig. 4.9 Profiles of the $r$-values predicted from the simulated and the experimental textures for a) the ULC steel, and b) the IF steel, c.r. 70% ($\Psi$ is the angle to the rolling direction).

4 Texture predictions in aluminium

The same four plasticity theories\(^{(1)}\) were used to predict texture evolution in several aluminium plates with different initial textures. In order to complement a study of grain subdivision in 40% cold-rolled aluminium (Chapter 5), the predictions of fcc rolling textures comprise both moderate (40%-50%) and high (60%-90%) thickness reductions. The reference materials consist of two commercial purity aluminium grades (AA1050) deformed in the lab, and two alloys (AA5182 and AA3104) provided by the industry. In all cases, the undeformed plate is recrystallised with average grain sizes up to 100 $\mu$m. However, the initial textures differ significantly.

The first reference material is a AA3104 plate that was cold rolled 55%, 76% and 89% (equivalent strains of 0.8, 1.4 and 2.2). The ODFs shown in Fig. 4.10a are derived from pole figure measurements by X-ray diffraction (XRD) performed in MTM. In the undeformed state, this material shows a very strong cube $\{001\}<100>$ texture (the ODF maximum is 22.8). The development of the $\beta$-fibre upon rolling is rather slow compared to the three other materials.

\(^{(1)}\) Obviously, for the fcc simulations, the twelve $\{111\}<110>$ slip systems were considered.
Fig. 4.10 ODFs representing the experimental aluminium textures. Contour lines: 1 / 2 / 4 / 8 / 16.
Fig. 4.10 (continued). Note that the ND-rotated copper $\{113\}<121>$ component reported by Hirsch et al (1987) is also highlighted ("NDCu").
The second material used as reference is a AA5182 plate that was cold rolled 50% and 70% (equivalent strains of 0.7 and 1.2). The ODFs shown in Fig. 4.10b are derived from XRD measurements carried out in MTM. The initial texture has two major components: a strong cube (ODF max = 9.9) and a weak brass \{110\}<112>. The cold rolled texture reveals a fairly stronger $\beta$-fibre than the two next materials. This can be attributed to the higher rolling reduction as well as the initially higher intensity at the brass orientation.

The ODFs shown in Fig. 4.10c correspond to an AA1050 plate prepared in the Risø National Laboratory (Denmark). Samples corresponding to 40% as well as 60% thickness reductions were provided. The 40% cold rolled samples also serve for the OIM study of grain subdivision presented in Chapter 5. Due to the large and heterogeneous grain sizes (the average initial grain diameter is 100µm), it was impossible to cover a statistically representative sampling of grains in a single XRD pole figure measurement or a single OIM map. The textures used here are thus the average of several measurements performed in the mid-thickness rolling plane. These measurements were carried out in Risø as well as MTM. The undeformed plate has a weak cube texture (ODF max = 6.5). Upon rolling, the $\beta$-fibre builds up slowly. Remnants of the original cube component are definitely still present, spreading between RD-rotated cube \{025\}<100> and TD-rotated cube \{205\}<502>.

The second AA1050 plate was provided by S. Kalidindi and his collaborators at the Drexel University (USA). Here, the starting texture is almost random and the plate is compressed in a channel-die up to 40% thickness reduction. The $\beta$-fibre develops more clearly than in all other plates, with a maximum at copper \{112\}<111>. The corresponding ODFs are presented in Fig. 4.10d. They are the averages of several OIM measurements carried out in Drexel and are fairly similar to XRD results reported by Panchanadeeswaran and Field (1995) about a cold rolled aluminium plate having also a random starting texture.

In conclusion, the four initial textures mainly differ by the strength of the cube \{001\}<100> component that decreases from the first to the last material presented. Applying the procedure for characterising quantitatively the cube-fibre and the $\beta$-fibre (section 1), the following trends are revealed:

- Fig. 4.11 shows the profiles of ODF-intensity integrals computed in sections perpendicular to the fibres. In all materials considered, rolling has the effect of reducing the volume fraction of grains having orientations along the cube-
fibre whereas the volume fraction of grains oriented along the β-fibre increases. It also appears that the formation of the β-fibre is faster in materials having a weaker initial texture such as the AA1050 received from Drexel. In this case, the values of the ODF-intensity integrals are distributed less evenly along the β-fibre, than in the plates having a strong cube texture at start (AA5182 and AA3104). Note that the same conclusion was drawn from the profiles of the ODF-intensities along the fibre centre-line but these profiles are not shown in order to save space.

- In Fig. 4.12, we observe that the β-fibre comes closer to its theoretical location with increasing strain. For example, there is a progressive shift from the \{4 4 11\}<11 11 8> component at \( (\phi_1=90^\circ, \Phi=27^\circ, \phi_2=45^\circ) \) towards copper \( (\Phi=35^\circ) \). This shift was also reported by Hirsch and Lücke (1988). It is also remarkable that the β-fibre is more distant from its theoretical position (up to \( \sim 10^\circ \)) in the AA1050 plates with a weak initial texture than in the AA5182 and AA3104 plates having a strong initial cube \(^{(1)}\).

This analysis reveals a correlation between strength of the cube component in the initial texture and the rolling texture \(^{(2)}\). When applying the various plasticity models, we will check whether this effect is captured and we will study the orientation path predicted for individual grains. Hirsch et al (1987) have found that grains oriented initially near cube can produce different texture components after rolling. According to them, certain near-cube grains rotate first around RD towards Goss \{011\}<100> then around ND towards brass, whereas other near-cube grains rotate around ~TD, forming TD-rotated cube \{205\}<502> and bridging cube and copper via ND-rotated copper \{113\}<121> \((\phi_1=73^\circ, \Phi=25^\circ, \phi_2=45^\circ)\). The latter components have seldom been reported. They are, however, clearly depicted in the ODFs of the AA1050 plate received from Risø (Fig. 4.10c), in the ODFs of the AA3104 plate (to a lesser extent), and in some previous studies (Engler, 1996; Samajdar et al, 1999).

\(^{(1)}\) The β-fibre is too weak to be recognised in the 40% c.r. AA1050 plate from Risø (the nearby rotated cube component yields the maximum ODF intensity in many sections perpendicular to the β-fibre).

\(^{(2)}\) This correlation should be verified by further investigations. It is likely that the initial texture is not the unique cause of the differences observed after cold rolling. Indeed, the reference aluminium plates each have a different purity and processing route (industry/lab). Furthermore, the ODFs were measured by different techniques.
Fig. 4.11 Characterisation of the experimental aluminium textures
ODF-intensity integrals in sections of the cube- and the β-fibres.
RDC={025}<100>, Cube={001}<100>, TDC={205}<502>,
Brass={110}<112>, S={123}<634> and Copper={112}<111>. 
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Fig. 4.11 (Continued)
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The four previously presented plasticity models have been applied to the texture predictions in the aluminium plates. In order to save space and because texture predictions are not so different from one aluminium plate to the other, not all predicted ODFs are inserted in the text. Fig. 4.13 presents the ODFs predicted for two plates at moderate strains (40% and 55% CR) and Fig. 4.14 corresponds to the two other plates and to higher strains (60% and 70% CR). To allow for a direct comparison, the ODFs predicted using the new version of the LAMEL model are also shown, although this model will only be described in Section 4.

The predicted textures have been characterised in a similar way as the experimental textures. In Fig. 4.15, the various model predictions are evaluated by analysing the profiles of the ODF-intensity integrals calculated in successive sections perpendicular to the cube-fibre and to the β-fibre. According to the method chosen for characterising the textures, the position of the cube-fibre is always the same, but the position of the β-fibre may vary from one texture to the other. However, in some predicted textures, the maximum ODF intensity in the section $\phi_2=90^\circ$ is not brass, but RD-rotated cube or Goss. This is for example the case of the textures predicted using the pancake model and the LAMEL model. For these textures, locating the β-fibre with the procedure proposed in Section 1 does not make sense because there is no local maximum near brass; the only maximum in the ODF section is RD-rotated cube. Fig. 4.16 shows the profiles that one would obtain by applying the texture

![Fig. 4.12 Exact location of the β-fibre in $\phi_2=\text{cst.}$ sections of the experimental fcc textures.](image-url)
characterisation procedure without a sense of critics. According to Fig. 4.16c, the pancake model predicts almost exactly the ODF intensity of brass, whereas Fig. 4.13 shows that this intensity is actually measured along the cube-fibre. To avoid such misinterpretations, the profiles of ODF-intensity integrals shown in Fig. 4.15 are computed by systematically checking that the skeleton-line identified by the automatic procedure was distant from the experimental \( \beta \)-fibre by less than 15°. If this was not the case, the predicted profile was recalculated at the location found for the corresponding experimental texture. In general, this was not necessary for the FC Taylor model, the FE model and the new LAMEL model. Integrals have the advantage that they are not so sensitive to small shifts of the \( \beta \)-fibre location and that they better correspond to volume fractions than the single ODF-intensities. From the profiles presented in Fig. 4.15, the following preliminary conclusions can be drawn about the various models:

- The FC Taylor model predicts rolling textures with much too high ODF-intensities close to the \( S \) and copper components. Furthermore, for the textures having a strong initial cube component, the volume fraction of grains oriented near cube does not decrease fast enough in the predictions.

- The RC pancake model yields very bad texture predictions. The greatest discrepancy relative to the experimental textures is the extremely high volume fraction of grains oriented between RD-rotated cube and Goss whereas brass is completely absent from the predictions.

- The LAMEL model yields predictions that are midway between the predictions of the FC Taylor and the RC pancake model. These predictions are thus worse than the predictions of the classical FC Taylor model.

- The predictions obtained with the FE model are better than for the Taylor FC model. In general, lower volume fractions are predicted close to \( S \) and copper (but still too high compared to the experimental textures). The strength of the components oriented along the cube-fibre is better reproduced. The FE model also better predicts the location of the \( \beta \)-fibre than the other models.

All plasticity models predict that grains oriented initially near cube undergo either zero rotation (because slip is distributed evenly among symmetric slip systems) or rotate around RD towards Goss. The formation of the \( TD \)-rotated cube and \( ND \)-rotated copper components, which was observed experimentally (see page 75), is captured by none of the applied models.
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Fig. 4.13 Comparison of the experimental ODF measured in the AA1050 c.r. 40% (from Drexel) and in the AA3104 c.r. 55%, to the ODFs predicted by various texture models. Contours: 1 / 2 / 4 / 8.
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Fig. 4.13 (Continued).
Fig. 4.14 Comparison of the experimental ODF measured in the AA1050 c.r. 60% (from Risø) and in the AA5182 c.r. 70%, to the ODFs predicted by various texture models. Contours: 1 / 2 / 4 / 8 / 16 / 25.
Fig. 4.14 (Continued).
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Fig. 4.15a Strength of the cube- and β-fibres: AA1050 from Drexel (CR 40%).

Fig. 4.15b Strength of the cube- and β-fibres: AA1050 from Risø (CR 40%).

Fig. 4.15c Strength of the cube- and β-fibres: AA3104 (CR 55%).
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Fig. 4.15d Strength of the cube- and β-fibres: AA1050 from Risø (CR 60%).

Fig. 4.15e Strength of the cube- and β-fibres: AA5182 (CR 70%).

Fig. 4.15f Strength of the cube- and β-fibres: AA3104 (CR 90%).
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The various plasticity models have also been compared by computing the texture index of the difference between the predicted ODFs and the experimental ones (Table 3). This confirms the impression that we had after the quantitative analysis of the fibres: the FE model gives the best texture predictions, followed by the FC Taylor model. The textures predicted by the LAMEL model and the RC pancake model do not match the experimental textures at all.

Fig. 4.16 Characterisation of the β-fibre that is predicted by the various models for the AA5182 plate CR 70%. a) Exact location of the fibres; b) intensity along the skeleton line of the predicted fibres.
Table 3  Comparison of the texture predictions in aluminium, relying on the texture index of the difference relative to the experimental texture. (1)

<table>
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<td>(Drexel)</td>
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<tr>
<td>AA1050</td>
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<td>2.89</td>
<td>1.04</td>
<td>0.44</td>
<td>0.82</td>
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<td>(Riso)</td>
<td>60%</td>
<td>1.83</td>
<td>4.82</td>
<td>2.22</td>
<td>1.40</td>
<td>1.47</td>
</tr>
<tr>
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<td>70%</td>
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<td>4.31</td>
<td>1.17</td>
<td>0.68</td>
<td>0.86</td>
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<tr>
<td>AA3104</td>
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<td>1.50</td>
<td>0.63</td>
<td>0.87</td>
</tr>
<tr>
<td></td>
<td>90%</td>
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<td>6.81</td>
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<td>1.77</td>
<td>2.12</td>
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(1) All texture indexes are computed with LMAX= 32.

The different texture predictions can also be evaluated by calculating for each of them the profiles of $r$-values that correspond to tension tests on samples cut in various directions in the plane of the plate. The results are shown in Fig. 4.17 for two of the materials investigated. They are consistent with the previous remarks.

Fig. 4.17  Profile of the $r$-value calculated for the textures predicted from the various texture models.
In section 2.2, a new procedure has been introduced for solving the Taylor ambiguity. The development of this procedure was motivated by the fact that the previously used method gave rise to lack of convergence when the stress state corresponded to a rib or a facet of the yield locus. This is often the case in the LAMEL model (see Fig. 3.2 in Chapter 3) and even more in RC models.

A second advantage of the new routine for solving the Taylor ambiguity is that it allows different choices to be made among the energetically equivalent solutions. Experience has shown that this was only relevant when applying the FC Taylor model (where the ambiguity is greatest because all solutions are corner solutions (1)). For fcc and applying FC Taylor, the best texture predictions were obtained by selecting the valid solution that minimises the expression given in Eq. 4.3. This is illustrated in Fig. 4.18-19, by comparing predictions that are obtained using the cited criteria, its inverse (maximisation of Eq. 4.3), or when the arithmetic average of all valid solutions is taken. Texture development is slower when minimising Eq. 4.3, than when applying the two other criteria. In fact, minimising Eq. 4.3 distributes slip on as many slip systems as possible, leading to a small lattice rotation rate in each individual grain. The latter can be concluded from Eq. 1.3: the amplitude of \( \Omega_{ij}^L \) is smaller if all critically stressed slip systems (1) are active than if the same amount of dislocations would glide predominantly along one or two of these slip systems.

However, solving Taylor ambiguity in this way contradicts experimental observations: the formation of slip lines and dislocation patterns can often be related to the one or the two most active slip systems, which tends to indicate that slip is restricted to as few slip systems as possible. The improvement of the texture predictions might thus be accidental. Probably, the final grain orientation predicted by applying FC Taylor and distributing slip on 6 or 8 slip systems is never produced in the real material. Nevertheless, this final grain orientation might correspond approximately to the average of all final orientations arising when grains with the same initial orientation interact with different neighbours, which would explain why the FC Taylor model performs rather well when considering only the global texture evolution.

Finally, it must be reminded that Taylor ambiguity disappears when the slip resistance \( (\tau_s) \) is different for each slip system. Taylor ambiguity can thus be

---

(1) Under fcc slip, 6 or 8 slip systems are critically stressed at corners of the yield locus.
solved in a more physically sound way by implementing slip system hardening due to dislocation interaction (Peeters et al., 2001; Seefeldt et al., in press).

Fig. 4.18 Prediction of 70%CR starting from a random texture and applying different criteria for solving the Taylor ambiguity. a) Minimisation of Eq. 4.3; b) arithmetic average of all valid solutions; c) Maximisation of Eq. 4.3.

Fig. 4.19 Integral skeleton lines showing the effect of applying different criteria for solving the Taylor ambiguity. (Same ODFs as Fig. 4.18.)
A surprising outcome of the last section is that the LAMEL model, which gave the best texture predictions under bcc slip, did not at all repeat this performance under fcc slip. Actually, its predictions under fcc slip are even worse than those of the FC Taylor model that does not consider interactions of the grain with a specific neighbourhood. The $l_{13}$ and $l_{23}$ shears, which are fully relaxed when applying the RC pancake model, and partly relaxed for the LAMEL model, appear to have a very detrimental effect on fcc texture predictions. The most significant discrepancy with regard to the experimental textures is the too low ODF intensity that is predicted for the brass $\{110\}<112>$ component.

From the study of Aernoudt and Stüwe (1970), one knows that brass-oriented grains have a strong tendency to undergo $l_{12}$ (RD-TD) shear, and that such shear improves the component’s stability during plane strain compression. This increased stability of the brass component can be demonstrated by simulating plane strain compression for all possible orientations in Euler space, and then highlighting the orientations that have rotated towards brass (Fig. 4.20). The three spherical boxes defined in Fig. 4.20a contain lattice orientations that are, respectively, within 5°, 10° and 15° of the brass orientation. The orientations predicted to rotate within these boxes (after a strain of 1.0) are indicated in Fig. 4.20b-d for the FC Taylor model and two RC models in which either $l_{12}$, or $l_{13}$ and $l_{23}$ (pancake model), are relaxed (1). It is clear that very few orientations rotate toward brass when the pancake model is used, conversely to what happens when the $l_{12}$ shear is relaxed (the boxes are much wider). Also noteworthy is the fact that, under FC Taylor, any orientation that is initially within 15° of brass remains within this range (or gets closer to brass) after a strain of 1.0. This is also true when $l_{12}$ is relaxed. However, the volume fraction of grains having such initial orientation may be very small in the experimental texture. It is thus interesting to perform a real texture prediction, using the RC model with $l_{12}$ relaxed, and to check whether the predicted ODF is any better than the results from the other models. This is not

(1) Obviously, such predictions cannot be performed for N-site models, such as the LAMEL and FE models, because the rotation of each grain also depends on the specific neighbourhood.
really the case as is illustrated in Fig. 4.21 for the AA5182 plate cold rolled 70%. Compared to the experimental texture (Fig. 4.14), the ODF intensity at brass is too high whereas the intensity at copper is too low. Furthermore, the maximum found in the section $\varphi_2=90^\circ$ of the predicted ODF is not brass \{110\}<112> (at $\varphi_1=35^\circ$ and $\Phi=45^\circ$), but rather \{110\}<111> (at $\varphi_1=55^\circ$ and $\Phi=45^\circ$). The latter component belongs to the <111>//RD fibre that would be produced by uniaxial tension along RD, but is absent of experimental rolling textures.

Fig. 4.20 Illustration of the stability of the brass component as predicted by various texture models. a) Definition of 3 spherical "boxes" around brass (5°, 10° and 15°). Orientations that are predicted to rotate within these boxes using: b) FC Taylor, c) RC pancake, and d) RC with the RD-TD shear relaxed.
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Fig. 4.21 Texture of the 70% cold rolled AA5182 plate as predicted by the RC model with $l_{12}$ relaxed. Predictions of other models in Fig. 4.14 (contours: 1 / 2 / 4 / 8).

The fact that a relaxation of $l_{12}$ yields too high ODF intensities at brass, is a hint that such shear is not fully relaxed in the real material. Indeed the volume misfit that can be induced by a relaxation of $l_{12}$ or $l_{23}$ is more important than for a $l_{13}$ relaxation (pancake model). After 50% thickness reduction of an initially equiaxed grain ($d \times d \times d$), the volume susceptible to cause geometrical misfit is $d^3/2$ for a unitary $l_{12}$ or $l_{23}$ shear, whereas it is only $d^3/4$ for a unitary $l_{13}$ shear (Fig. 4.22). Therefore the $l_{12}$ and $l_{23}$ shear might give rise to significant reaction stresses from the grain surrounding, and their complete relaxation cannot be justified as easily as for $l_{13}$.

Fig. 4.22 Geometrical misfit that is likely to be created by the relaxation of a) $l_{12}$ (top view), b) $l_{13}$ (side view), and c) $l_{23}$ (front view).
In Chapter 3, we have seen that shear relaxations within a grain can be partly constrained by imposing that there is no grain boundary sliding at the interface with an adjacent grain (LAMEL model). Therefore, it seems appropriate to introduce the \( l_{12} \) shear as a supplementary partial relaxation in the LAMEL model. This is illustrated in Fig. 4.23, also showing that the no-boundary-sliding condition here implies that the two interacting grains undergo the same \( l_{12} \) shear (denoted Type III in the figure). The volume that is susceptible to cause geometrical misfit is smaller than in Fig. 4.22, but it is still more important for Type III and Type II (\( l_{23} \) shear) relaxations than for Type I (\( l_{13} \) shear).

![Fig. 4.23 Illustration of the three types of shear considered by the new version of the LAMEL model (1=RD, 2=TD, 3=ND).]

The mathematics involved with the introduction of a Type III relaxation in the LAMEL model are fairly obvious. One variable must be introduced in the equations, which is the “pseudo slip system” representing the supplementary relaxation. There is one supplementary degree of freedom relative to the old version of the LAMEL model, which means that \( 10 - 3 = 7 \) slip systems need to be activated to achieve the imposed deformation in two grains. Note also that the solution of the energy minimisation will be such that the 2 grains have opposite \( \sigma_{12} \) stress.

The texture predictions obtained with the new LAMEL model on aluminium rolling textures have been presented in the previous section. One observes a significant improvement compared to the predictions of the original LAMEL model. The intensity at the brass component is, however, too high. This may indicate that, in the real material, the reaction stresses against \( l_{12} \) (and \( l_{23} \)) are stronger than those against \( l_{13} \), which can be justified from Fig. 4.22. Also remarkable is the fact that the brass component is found to be stronger in cold rolled copper where deformation bands arise perpendicular to TD (see Fig.
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2.6 taken from Lee and Duggan (1993)) and could undergo opposite RD-TD shears with little geometrical misfit at the grain boundary (see Fig. 3.4)

It should finally be mentioned that the new LAMEL model leads to marginal differences compared to the original LAMEL model, when cold rolling textures are predicted in steel.

6 Discussion

The results presented in this chapter demonstrate that textures predictions in cold rolled steel and aluminium plates are significantly improved when each grain is considered to interact with a specific neighbourhood. The analysis was conducted on a variety of materials with distinct initial textures, involving moderate as well as high strains. The evaluation of the simulated textures relied on a new technique for quantitative texture characterisation. Without exception, the experimental textures were more closely reproduced by applying the FE model or the LAMEL model (in its revised form) than by applying classical plasticity theories.

This important conclusion convinces us of the necessity to apply $N$-site interaction models in all future studies of the texture development during rolling. For example, when investigating how some process parameters influence the final rolling texture, or when estimating the creation of texture gradients through the plate thickness, etc.

It is likely that $N$-site interaction models distribute stresses and strains among the crystallites in a more correct way than the classical theories do. In order to ascertain this statement, the predictions should nevertheless be evaluated not only from a macroscopic viewpoint (as was done so far), but also at the scale of individual grains. The purpose of the next two sections is to extract such local information from the various simulation results. Then, in Chapter 6, an attempt will be made to predict grain subdivision with the LAMEL model and with the FE model, which is another means of evaluating how the models perform at the grain level.

6.1 Local deformation tensor

In the FE element simulations, all components of the local deformation tensor $F_{ij}$ are susceptible to vary over the mesh representing the polycrystal. This condition is required for the combined fulfilment of stress equilibrium and
strain compatibility. In RC theories and in the LAMEL model, these conditions are not satisfied: it is assumed for simplicity that only $F_{13}$, $F_{23}$ (and $F_{12}$ in the revised LAMEL model) differ from grain to grain.

It is interesting to compare the local $F_{ij}$ components that are predicted by the various models. In the Taylor-type models, $F_{ij}$ can be computed from the local velocity gradient $l_{ij}$ by integrating explicitly

$$l_{ij} = F_{ij}^{-1} \frac{\partial F_{ij}}{\partial t}. \quad (4)$$

This yields $\Sigma l_{ij}\Delta t = \ln(F_{ij})$, or $F_{ij} = \exp(\Sigma l_{ij}\Delta t)$. The latter expression must be calculated numerically:

$$F_{ij} \approx \sum_{k=1,n} \left(\frac{\Sigma l_{ij}\Delta t}{k!}\right)^k \quad \text{(with e.g. } n=10). \quad (5)$$

After 70% plane strain compression, the macroscopic deformation tensor is $F_{11}=3.3$, $F_{22}=1.0$, $F_{33}=0.3$ and $F_{12} = F_{21} = F_{13} = F_{31} = F_{23} = F_{32} = 0$. Although the local deformation tensor may deviate from these values, all used models predict that the macroscopic deformation is accomplished on average over the polycrystalline aggregate (1). In order to evaluate the amplitude of fluctuation of the local deformation tensor $F_{ij}$, the average of the absolute value of $F_{ij}$ can be calculated. This is done in Table 4 for the IF-steel and in Table 5 for the AA5182 aluminium.

The tables show only the components of $F_{ij}$ that are partly or fully relaxed in the Taylor-type simulations and have a macroscopic value equal to zero. According to the FE model, the normal components $F_{11}$, $F_{22}$, and $F_{33}$ fluctuate much less than the shear components. The tables allow making the following observations:

- All applied models predict the average $|F_{13}|$ and $|F_{12}|$ to be larger than the average $|F_{23}|$ (both in fcc and in bcc). Note that the difference in the volume

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\[1\] In the RC Taylor model and in the revised LAMEL model, this is ensured by the fact that the grain sampling represents an orthorhombic texture (i.e. mirror orientations are equally probable), and the fact that exactly opposite relaxations are predicted in grains with mirror orientations. In the FE simulations, the boundary conditions applied at the mesh outer surface guarantee that the average local deformation matches the macroscopic deformation.
susceptible to cause geometrical misfit (Fig. 4.22) seems not to play a major role here: on the one hand, the results are similar, independent of whether the corresponding reaction stresses are accounted for (FE model), or not (Taylor-type simulations). On the other hand, $|F_{13}|$ decreases more than $|F_{12}|$ when switching from LAMEL to FE (in steel), whereas the volume susceptible to cause misfit is larger for $F_{12}$, i.e. for RD-TD shears.

- The shear deformations predicted by the LAMEL model (the original and the new version) are approximately halfway between the fully relaxed shears predicted by the classical RC theories, and the shears predicted by the FE model. The reason why the shears are lower in the FE simulations than in the LAMEL model is likely to be related to the larger number of direct neighbours in the FE simulations. As each grain has six direct neighbours in the FE mesh, the chance is high that any significant deviation relative to the macroscopic deformation be impeded by important reaction stresses in at least one not-favourably-oriented neighbour. In the LAMEL model, large relaxations are more probable because they need to be accommodated by only one neighbour.

- The same trend is found if we base the comparison on the symmetric part of the local deformation tensor: $|F_{13} + F_{31}|$, $|F_{12} + F_{21}|$ or $|F_{23} + F_{32}|$. The values corresponding to the Taylor-type simulations are unchanged (as $F_{31}$, $F_{21}$ and $F_{12}$ are set to zero). In the FE model, $|F_{13} + F_{31}|$, $|F_{12} + F_{21}|$ and $|F_{23} + F_{32}|$ are almost equal to $|F_{13}|$, $|F_{12}|$ and $|F_{23}|$ respectively, which means that the local $F_{31}$, $F_{21}$ and $F_{32}$ components are much smaller than $F_{13}$, $F_{12}$ and $F_{23}$. This supports the choice made by the Taylor-type models (including the LAMEL model) to allow only pure-shear relaxations by setting $F_{31}$, $F_{21}$ and $F_{32}$ to zero.

Finally, it should be mentioned that FE simulations were carried out also with “brick-shaped” grains using 2 cubic elements per grain (Fig. 4.24). In this case, each grain has 10 direct neighbours instead of 6 previously and the local variables (stress, strain and dislocation slip) need not to evolve linearly across each grain along the rolling direction. However, this affected the local deformations only slightly (as indicated in Table 4 and in Table 5) and the effect on texture predictions was also negligible (not shown). More complex deformation patterns would be predicted if each grain was represented by at least ~10 finite elements and if the grain arrangement was less regular. However, the simulations would then require much larger computing time.
Table 4 Average absolute value of the local deformation tensor components (IF-steel cold rolled 70%)

|            | $|F_{12}|$ | $|F_{13}|$ | $|F_{23}|$ | $|F_{12} + F_{21}|$ | $|F_{13} + F_{31}|$ | $|F_{23} + F_{32}|$ |
|------------|----------|----------|----------|-------------------|-------------------|-------------------|
| RC Pancake | 0        | 0.96     | 0.37     | 0                 | 0.96              | 0.37              |
| Original LAMEL | 0 | 0.82     | 0.29     | 0                 | 0.82              | 0.29              |
| Only $l_{12}$ relaxed | 0.38 | 0        | 0        | 0.38              | 0                 | 0                 |
| New LAMEL  | 0.31     | 0.70     | 0.31     | 0.70              | 0.31              | 0.70              |
| FEM        | 0.26     | 0.41     | 0.17     | 0.29              | 0.40              | 0.19              |
| FEM bricks | 0.31     | 0.53     | 0.20     | 0.33              | 0.51              | 0.22              |

Table 5 Average absolute value of the local deformation tensor components (AA5182 cold rolled 70%)

|            | $|F_{12}|$ | $|F_{13}|$ | $|F_{23}|$ | $|F_{12} + F_{21}|$ | $|F_{13} + F_{31}|$ | $|F_{23} + F_{32}|$ |
|------------|----------|----------|----------|-------------------|-------------------|-------------------|
| RC Pancake | 0        | 1.25     | 0.17     | 0                 | 1.25              | 0.17              |
| Original LAMEL | 0 | 0.57     | 0.12     | 0                 | 0.57              | 0.12              |
| Only $l_{12}$ relaxed | 1.12 | 0        | 0        | 1.12              | 0                 | 0                 |
| New LAMEL  | 0.74     | 0.58     | 0.13     | 0.74              | 0.58              | 0.13              |
| FEM        | 0.39     | 0.39     | 0.06     | 0.41              | 0.38              | 0.07              |
| FEM bricks | 0.44     | 0.39     | 0.07     | 0.45              | 0.38              | 0.08              |

6.2 Development of a microtexture

The principal characteristic of $N$-site plasticity theories is that the slip activity predicted for a grain is influenced by the lattice orientation of one or several of its neighbors. At the start of the simulation, the interacting grains have a random misorientation with respect to one another (1). However, during the simulation, the slip activities predicted for the interacting grains are correlated with each other, which may induce the build up of a characteristic

(1) In the LAMEL simulations, the pairs of interacting grains are selected at random among the orientation sampling that represents the initial texture. In the FE simulations, this same initial orientation sampling is distributed at random over the mesh.
misorientation between the grains. Obviously, the development of such “microtexture” is more probable when applying the LAMEL model than the FE model because the correlation between the slip activities is strongest when interactions involve only two grains at a time.

![Fig. 4.24 FE mesh with brick-shaped grains. Each grain is represented by two cubic elements aligned with RD and has 10 direct neighbours instead of 6.](image)

It turns out that the LAMEL model predicts a significant development of microtexture. A first way to demonstrate this is to generate an ODF showing only the grains whose neighbours have a specific orientation. Such selection has been done after a simulation of 70% cold rolling on 10000 grains representing the ULC steel (Fig. 4.5). The ODFs shown in Fig. 4.25a-b (2) are produced, respectively, with the final and the initial orientations of grains whose neighbours have rotated within 15° of the E₁ orientation (1 1 1)[1 1 0]. It is clear that the lattice rotation predicted for these grains are strongly correlated with the lattice rotation of their neighbour: if one grain rotates towards E₁, the neighbour rotates towards E₂ (T T T)[T 1 0]. By adopting mirror orientations relative to the rolling plane, the interacting grains have the tendency to undergo opposite shears independent of the constraint imposed by the LAMEL model. The association of two grains with mirror orientations is the configuration

(2) Here, it is necessary to apply triclinic symmetry. Therefore the ODFs are presented with φ₁ ranging from 0° to 360° (instead of 0° to 90° under orthorombic symmetry).
leading to the largest LAMEL-type relaxation because opposite shears reduce the dissipated energy in both grains. Note that the formation of this microtexture could not be foreseen from the theoretical definition of the LAMEL model.

The same kind of trend was observed for grains with other orientations than $E_1$/$E_2$. However, the correlation was not as strong for these other orientations. This is illustrated in Table 6 based on a simulation of 70% cold rolling with the LAMEL model and starting from a random texture for both bcc and fcc (10000 grains). The development of microtexture is characterised by computing the texture index (T.I.) of the difference between two ODFs. The first ODF represents all 10000 grains, and the second ODF represents only the grains whose neighbours are oriented close to a characteristic orientation (as defined in Fig. 4.1 for bcc and Fig. 4.3 for fcc). In the absence of any microtexture, these two ODFs should be very similar and the T.I. of their difference should be ~0. This is evidently not true here.

As grains were expected to adopt mirror orientations, we have also estimated the strength of the microtexture by comparing the number of pairs in which the interacting grains had mirror orientations $N_{\text{mirror}}$ (e.g. $E_1$ for one and $E_2$ for the other) to the number of pairs in which the two grains had the same orientation $N_{\text{same}}$ (e.g. $E_1$ for both). If the interacting orientations were not
correlated, \( N_{\text{mirror}} \) should be equal to \( N_{\text{same}} \). This is because grains with mirror orientations have the same number of occurrences in the final grain sampling (e.g. number of grains with \( E_1 \) orientation = number of grains with \( E_2 \) orientation). In Table 6, we observe that \( N_{\text{mirror}} \) is generally not equal to \( N_{\text{same}} \). Grains with the \( E \) or the \( \text{brass} \) orientation are more often associated with their mirror orientation \( (N_{\text{mirror}}>>N_{\text{same}} \cdot \text{(multiplicity-1)}) \), whereas grains with the \( I \) or the \( \text{copper} \) orientation show opposite behaviour: they seem to avoid being associated with their mirror orientation \( (N_{\text{mirror}}<<N_{\text{same}} \cdot \text{(multiplicity-1)}) \).

The same simulations have been performed using the new version of the LAMEL model (including RD-TD shear relaxations). In Table 7, we can check that the development of microtexture is different and somewhat stronger in this case. The \( E \) and the \( S \) orientations are almost always associated with their mirror orientation, whereas the opposite trend is found for the \( I, F, \text{brass} \) and \( \text{copper} \) orientations. It is noteworthy that the \( \text{brass} \) orientation shows opposite behaviour when RD-TD shear is allowed or not allowed (i.e. using the original or the new version of the LAMEL model).

It is evident that the microtexture is not expected to be so strong in the real material, where grains have more than one direct neighbour. However, the situation considered by the LAMEL model could be approached at high strains if grains would form very flat lamellas with alternating orientations. In this case, grains could be considered to interact only with their bottom and top neighbours, which would bear the same orientation. This was already suggested in Chapter 3 (section 3.2) for simulating subdivision into deformation bands.

It would be worthwhile investigating experimentally (e.g. by OIM) whether lamellas with alternating orientations are formed and whether such bands bear

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(1) In fact, this statement is only valid for texture components having a single mirror orientation, which is the case of all considered orientations excepted \( H \) (bcc) and \( S \) (fcc). In an orthorombic texture, each orientation has up to 3 equivalents that are generated by applying mirror symmetries relative to the RD-TD plane ("rolling plane"), the RD-ND plane and the TD-ND plane. However, when one of these reference planes matches accidentally a symmetry plane of the cubic crystal lattice, i.e. a \{100\} plane or a \{110\} plane, the "multiplicity" of the orientation is reduced. This happens at \( H (<100>/ND \& <110>/RD) \), \( I (<110>/RD) \), \( E (<110>/RD) \) and \( F (<110>/TD) \) in steel, as well as \( \text{brass} (<110>/ND) \) and \( \text{copper} (<110>/TD) \) in aluminium. Therefore, \( I, E, F, \text{brass} \) and \( \text{copper} \) each have only one mirror orientation, whereas \( H \) has none and \( S \) has 3.
mirror orientations. This would convince us of the validity of the LAMEL assumptions for predicting local deformations at the grain scale. The OIM investigations of the next chapter do not allow drawing any conclusion about this question. Indeed, the performed OIM scans focus on the grain subdivision mechanisms and therefore require (i) a moderate strain (40% reduction) and (ii) a small step size. We believe that the microtexture, if it exists, could only be observed when grains are more flattened (at larger strains) and by scanning larger sample surfaces. This will be the object of future research.

Table 6 Development of a microtexture during the LAMEL simulations.

<table>
<thead>
<tr>
<th>Miller indices</th>
<th>T.I. of the ODF difference</th>
<th>N_{mirror}</th>
<th>N_{same}</th>
<th>N_{mirror} / N_{same (multi-1)}</th>
</tr>
</thead>
<tbody>
<tr>
<td>H (0 0 1)[1 1 0]</td>
<td>0.51</td>
<td>/</td>
<td>106</td>
<td>/</td>
</tr>
<tr>
<td>I_1 (1 1 2)[1-1 0]</td>
<td>1.86</td>
<td>80</td>
<td>144</td>
<td>0.55</td>
</tr>
<tr>
<td>I_2 (-1-1-2)[1-1 0]</td>
<td>1.89</td>
<td>80</td>
<td>166</td>
<td>0.48</td>
</tr>
<tr>
<td>E_1 (1 1 1)[1-1 0]</td>
<td>5.83</td>
<td>261</td>
<td>0</td>
<td>Infinite</td>
</tr>
<tr>
<td>E_2 (-1-1-1)[1 1 0]</td>
<td>4.84</td>
<td>261</td>
<td>0</td>
<td>Infinite</td>
</tr>
<tr>
<td>F_1 (1 1 1)[1 1-2]</td>
<td>2.14</td>
<td>109</td>
<td>76</td>
<td>1.43</td>
</tr>
<tr>
<td>F_2 (-1-1-1)[1 1-2]</td>
<td>2.23</td>
<td>109</td>
<td>104</td>
<td>1.05</td>
</tr>
<tr>
<td>Brass_1 (1 1 0)[1-1 2]</td>
<td>0.37</td>
<td>48</td>
<td>28</td>
<td>1.71</td>
</tr>
<tr>
<td>Brass_2 (-1-1 0)[1-1 2]</td>
<td>0.39</td>
<td>48</td>
<td>30</td>
<td>1.60</td>
</tr>
<tr>
<td>S_1 (1 2 3)[6 3-4]</td>
<td>1.52</td>
<td>576</td>
<td>226</td>
<td>0.85</td>
</tr>
<tr>
<td>S_2 (-1-2-3)[6 3-4]</td>
<td>1.56</td>
<td>592</td>
<td>200</td>
<td>0.99</td>
</tr>
<tr>
<td>S_3 (1 2 3)[-6-3 4]</td>
<td>1.44</td>
<td>584</td>
<td>176</td>
<td>1.11</td>
</tr>
<tr>
<td>S_4 (-1-2-3)[-6-3 4]</td>
<td>1.56</td>
<td>605</td>
<td>174</td>
<td>1.16</td>
</tr>
<tr>
<td>Copper_1 (1 1 2)[1 1-1]</td>
<td>1.80</td>
<td>225</td>
<td>362</td>
<td>0.62</td>
</tr>
<tr>
<td>Copper_2 (-1-1-2)[1 1-1]</td>
<td>2.05</td>
<td>225</td>
<td>440</td>
<td>0.51</td>
</tr>
</tbody>
</table>

(1) The total number of pairs is 5000.
Table 7 Development of a microtexture during the simulations with the LAMEL model in its revised form.

<table>
<thead>
<tr>
<th></th>
<th>Miller indices</th>
<th>T.I. of the ODF difference</th>
<th>$N_{\text{mirror}}$</th>
<th>$N_{\text{same}}$</th>
<th>$N_{\text{mirror}} / N_{\text{same}}(\text{mult-1})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>(0 0 1)[1 1 0]</td>
<td>0.60</td>
<td>/</td>
<td>138</td>
<td>/</td>
</tr>
<tr>
<td>$I_1$</td>
<td>(1 1 2)[1-1 0]</td>
<td>1.92</td>
<td>105</td>
<td>138</td>
<td>0.76</td>
</tr>
<tr>
<td>$I_2$</td>
<td>(-1-1-2)[1-1 0]</td>
<td>1.78</td>
<td>105</td>
<td>142</td>
<td>0.74</td>
</tr>
<tr>
<td>$E_1$</td>
<td>(1 1 1)[1-1 0]</td>
<td>6.50</td>
<td>290</td>
<td>0</td>
<td>Infinite</td>
</tr>
<tr>
<td>$E_2$</td>
<td>(-1-1-1)[1 1 0]</td>
<td>5.66</td>
<td>290</td>
<td>0</td>
<td>Infinite</td>
</tr>
<tr>
<td>$F_1$</td>
<td>(1 1 1)[1 1-2]</td>
<td>2.79</td>
<td>44</td>
<td>132</td>
<td>0.33</td>
</tr>
<tr>
<td>$F_2$</td>
<td>(-1-1-1)[1 1-2]</td>
<td>2.93</td>
<td>44</td>
<td>124</td>
<td>0.35</td>
</tr>
<tr>
<td>Brass1</td>
<td>(1 1 0)[1-1 2]</td>
<td>2.73</td>
<td>73</td>
<td>182</td>
<td>0.40</td>
</tr>
<tr>
<td>Brass2</td>
<td>(-1-1 0)[1-1 2]</td>
<td>2.62</td>
<td>73</td>
<td>152</td>
<td>0.48</td>
</tr>
<tr>
<td>$S_1$</td>
<td>(1 2 3)[6 3-4]</td>
<td>2.43</td>
<td>423</td>
<td>16</td>
<td>8.81</td>
</tr>
<tr>
<td>$S_2$</td>
<td>(-1-2-3)[6 3-4]</td>
<td>2.55</td>
<td>448</td>
<td>12</td>
<td>12.4</td>
</tr>
<tr>
<td>$S_3$</td>
<td>(1 2 3)[-6-3 4]</td>
<td>2.70</td>
<td>435</td>
<td>6</td>
<td>24.1</td>
</tr>
<tr>
<td>$S_4$</td>
<td>(-1-2-3)[-6-3 4]</td>
<td>2.66</td>
<td>428</td>
<td>12</td>
<td>11.9</td>
</tr>
<tr>
<td>Copper1</td>
<td>(1 1 2)[1 1-1]</td>
<td>2.70</td>
<td>41</td>
<td>178</td>
<td>0.23</td>
</tr>
<tr>
<td>Copper2</td>
<td>(-1-1-2)[1 1-1]</td>
<td>2.51</td>
<td>41</td>
<td>194</td>
<td>0.21</td>
</tr>
</tbody>
</table>
CHAPTER 5: STATISTICAL STUDY OF THE HETEROGENEITY OF GRAIN SUBDIVISION IN ROLLED ALUMINIUM

Through the presentation of plasticity theories, the literature review about grain subdivision mechanisms and the comparative evaluation of texture prediction models, we have gathered convincing proofs that grain interactions play an important role in the micromechanics of cubic metals. However, as we stressed already in Chapter 2, the yet available experimental results do not provide complete answers about the extent to which grain interactions trigger the formation of in-grain orientation spreads and the fragmentation of the grain. Not so much is known, either, about the correlation existing between the orientation of a grain and the type/level of subdivision in this grain.

The purpose of the study that is to be presented now is to provide supplementary information about the heterogeneity of grain subdivision that occurs during cold rolling of aluminium. The study relies on a new powerful technique for measuring local lattice orientations in the SEM: Orientation Imaging Microscopy (OIM). This technique permits an automatic mapping of large sample surfaces compared to TEM. This is useful in two respects: (i) the intra-granular orientation spread can be observed over representative grain sections, and (ii) large maps enable an analysis of tendencies that can only be derived from the averaged behaviour of many grains. In the first section, the technique and the data acquisition procedure are described. Then, orientation maps are compared to pre-existing TEM pictures of the same material and the quality of the observations is discussed. Finally, a computational procedure is proposed for exploiting the OIM data in a study of the correlation between the mean orientation of a grain and the type and level of subdivision.
1 Description of the OIM technique

Orientation Imaging Microscopy (OIM) (Adams et al, 1993), also termed Automated Crystal Orientation Mapping (ACOM) (Schwarzer, 1997), is today’s most convenient tool for spatially resolved microtexture analysis. In OIM and ACOM, local crystallographic orientations are measured in a Scanning Electron Microscope (SEM) by focusing the beam to a fine spot within a grain, and analysing the electron back-scattering diffraction (EBSD) pattern (Dingley and Randle, 1992). The EBSD pattern is captured on a phosphor screen near the sample, and it is recorded by an ultra-sensitive camera positioned behind the screen and outside the chamber (see Fig. 5.1). In order to raise the intensity of diffracted electrons reaching the screen, the sample is tilted of ~70° towards the screen.

Fig. 5.1 Schematic representation of the OIM installation.

An EBSD pattern is constituted by a superposition of bands (see Fig. 5.2), each stemming from a family of diffracting crystallographic planes. The intersection of two bands thus indicates a crystal direction. The thickness of a
band is proportional to the Bragg angle (the crystal-plane spacing) and its position on the screen relates to the lattice orientation to be determined. In cubic metals, it is sufficient to identify three crystal directions on the phosphor screen to be able to derive the lattice orientation of the diffracting volume \(^{(1)}\). The mathematical treatment involved in the band recognition and the orientation calculation is commonly called “pattern indexing”. It is automatically carried out by a computer interfaced to the microscope and it requires less than a second per pattern. The same computer is used for automatically displacing the incident electron beam along a grid on the sample surface, resulting in so-called orientation maps that cover large sample areas compared to the TEM studies cited in Chapter 2.

A limitation of OIM is that it requires a very clean surface, and that lattice imperfections, such as dislocations and inclusions, interfere with the formation of the EBSD pattern. If the diffraction volume contains too many imperfections, shadows appear on the phosphor screen, some diffraction bands become unrecognisable and pattern indexing may be impeded. This means (i) that the deformed layer created during mechanical polishing of the sample surface must be removed by electropolishing, and (ii) that samples rolled to high strains cannot be investigated by OIM due to the too low dislocation spacing. Various

\(^{(1)}\) This constitutes a fundamental difference compared to texture measurements by X-ray diffraction. In the latter case, the Bragg angle is fixed by the goniometer setting, and the diffracted intensity that is recorded by the detector arises from only one crystal plane family. X-ray diffraction thus yields incomplete information about the lattice orientation, and pole figure inversion is required to compute the ODF.
Chapter 5 Statistical study of the heterogeneity of subdivision

Mathematical methods have been developed to improve the chances of a correct indexing, even when the diffraction pattern is incomplete. A “confidence index” (CI) is used to detect and withdraw wrongly indexed patterns, whereas a parameter termed “image quality” (IQ) indicates how “clean”, i.e. free of dislocations, the crystal lattice is. The IQ is actually a measure of the band contrast and is fairly sensitive to the local dislocation content (as illustrated in the next section).

Typical applications of the OIM technique are the study of spatial heterogeneities of the texture, correlations between grain size and grain orientation, statistical studies of misorientations between adjacent grains (for example the formation of CSL boundaries during recrystallisation), phase identification in multiphase materials, etc. Surprisingly, OIM has so far relatively seldom been used to study fragmented structures in cold deformed materials (compared to the still abundant TEM work). It is true that the resolution of the OIM technique is limited, especially in strained materials, and that some of the micro-scale features may not be identified.

The resolution of the OIM technique is generally discussed in terms of spatial resolution and angular accuracy:

- The spatial resolution describes the smallest beam-sample interaction volume yielding sufficient diffracted intensity to produce indexable patterns. In conventional SEM systems with a W-filament, spatial resolutions of the order of 0.3-0.5 µm are reported. However, the spatial resolution varies with the material, and requires that the accelerating voltage and the beam current be fine-tuned in each case. As the sample surface is tilted of only ~20° relative to the incident electron beam, the diffracting volume is an ellipsoid that is elongated in the direction perpendicular to the tilt axis. Consequently, the angular resolution is ~3 times worse in this “longitudinal” direction (Isabell and Dravid, 1997; Humphreys et al, 1999). Furthermore, the spatial resolution can be significantly enhanced (~0.1 µm) by making use of a Field Emission Gun (FEG) SEM that allows higher current intensities to be focused on finer spots (Humphreys, 1999). As both SEM systems are available in our department, their performances have been compared.

- The second important parameter of OIM investigations is the angular accuracy of the local lattice orientation measurements. According to the literature, one may expect from EBSD measurements an absolute angular
accuracy of \( \sim 1^\circ \) and a relative angular accuracy (between two orientations in the same map) of \( \sim 0.5^\circ \) (Humphreys, 1999). The angular accuracy depends on the quality of the diffraction image transmitted to the computer, on the mathematical treatment used for pattern indexing and on the calibration of the OIM system. The quality of the diffraction image is a function of the camera resolution and of the success in eliminating the background that is created by inelastic electron scattering. The system calibration also plays a crucial role. It consists of the determination of 4 parameters that must inform the computer precisely about the distance and the orientation of the phosphor screen relative to the sample surface.

In the next section, the OIM technique is applied to the observation of a cold rolled aluminium plate. As we hope to resolve micrometer-sized grain fragments having misorientations of the order of \( 1^\circ \), both the spatial resolution and the angular accuracy should be critical.

2  Observation of a cold rolled aluminium plate by OIM

2.1  Material selection and sample preparation

The material selected for the OIM study has already served in Chapter 4 for testing the texture prediction models under fcc slip condition. It is a 1050 commercial purity aluminium provided by the Risø National Laboratory in Denmark. Its composition is (in weight %): 0.25 Fe, 0.13 Si, 0.03 Sb, 0.03 Ni, 0.02 Ti, 0.02 Cr, 0.01 Zn. Prior to cold rolling, the plate had a thickness of 10mm, it was recrystallised with a mean grain size of 100\( \mu \)m. Cold rolling to a thickness reduction of 40% was performed in one pass on lubricated rolls. The roll-gap geometry was observed to yield a rolling type texture throughout the plate body (Mishin et al, 2000).

It was a deliberate choice to test the OIM technique on a material of which the deformation structure had already been thoroughly investigated by TEM. Doing so, we can tell to what extent the limited resolution of OIM causes details to be missed. At this moderate strain, the spacing between dislocation walls is not too small, and the spatial resolution of a conventional SEM system should enable fairly complete orientation maps. However, as the angular accuracy of the technique is only \( \sim 1^\circ \), only subgrains with larger misorientations can be distinguished.
For later comparison with the OIM results, Fig. 5.3 presents an example of the deformation structure revealed by TEM. Intersecting extended dislocation boundaries are aligned at approximately \(+/-40^\circ\) to the rolling direction (RD). Individual cells forming cell blocks (CBs) are also clearly resolved. From measurements in the TEM, the misorientation between adjacent cells is known to be less than 1°, whereas CBs have misorientations between 1° and 15°.

Different types of specimen were prepared from the longitudinal section of the plate, i.e. from the section containing the normal direction (ND) and the rolling direction (RD):

- Bulk specimens were first polished mechanically to 3\(\mu\)m roughness. Then, they were polished electrochemically in a Struers A2 electrolyte (60ml H\(_2\)O, 300ml ethanol, 50ml 2-Butaxy ethanol and 40ml perchloric acid). The electropolishing temperature was 3-5°C, the voltage was \(\sim8V\), the distance to the aluminium cathode was 20-30mm, yielding a current of \(\sim5mA\). The time ranged between 2 and 2.5min (by trial and error).
In addition, thin foils that had been preliminarily inspected by TEM (in Risø) were pasted with a carbon sticker on a SEM sample holder for OIM investigation.

2.2 Experimental set-up for the OIM data acquisition

The OIM study was performed using a Philips XL30 scanning electron microscope with a Tungsten filament (1). The “beam control” mode was applied, i.e. the electron beam moved whereas the position of the stage was unchanged. The best OIM performance was obtained using a moderate accelerating voltage 12-15kV, but a large spot size corresponding to “spot 6.5-7” on the XL30 setting (2). The diffraction pattern was recorded by a CCD camera and the signal-to-noise ratio was enhanced by hardware background correction. Three examples of corrected diffraction patterns from this deformed material are presented in Fig. 5.2. These patterns shows relatively few bands but with a high contrast, which turned out to yield the best indexing statistics (and the best angular accuracy).

The TSL software was used for indexing EBSD patterns. This means that the orientation recognition was carried out as follow: (i) the computer identifies as many diffracting bands as possible. (ii) It computes the lattice orientation corresponding to either set of 3 bands (that do not intersect in just one point). (iii) If the answer is not unanimous, the preferred solution is the orientation receiving the largest number of “votes”. (iv) The probability of a correct indexing is estimated by a “confidence index” (C.I), that is equal to the difference in number of votes attributed, respectively, to the 1st and 2nd solution divided by the total number of votes. It turned out that only the measurements having a CI smaller than 0.1 needed to be rejected.

Sixteen OIM scans were performed in different regions of the various plate samples, spreading the investigated areas over large distances. On average, each map contains ~100,000 orientation measurements forming a hexagonal grid. This represents ~22 hours automatic scanning. The step size varied from 0.5µm to 1µm for different scans. In all, more than 400 grains were mapped.

---

(1) The Philips XL30 FEG microscope was used only once, for comparison.

(2) In the secondary electron image, such spots were observed to burn areas with diameter ~1µm. (The corresponding absorption current is unknown.)
2.3 Selected OIM results

2.3.1 Description of some characteristic orientation maps and comparison to the previous TEM results

Several representative orientation maps created using OIM are shown in Fig. 5.4-7. The orientation maps are produced with step sizes of 0.7-0.75\(\mu\)m and they cover 40-50 grains in the longitudinal (RD-ND) section of the plate. The colouring of the maps is related to the projection of either RD or ND in the inverse pole figure: regions with the same colour have the same crystal direction aligned with RD (or ND), but they do not necessarily have an identical lattice orientation. Black lines represent grain or subgrain boundaries that accommodate “large” misorientations (the value is specified in each figure caption). Such maps reveal both the “long-range” orientation gradients and the fragmentation of the grain.

To investigate the deformation structure in more detail, one intensely subdivided grain from Fig. 5.4 was repeatedly inspected with a smaller step size: 0.3\(\mu\)m (Fig. 5.5). In the latter case, the sample was rotated \(\sim40^\circ\) around the transverse direction (TD) to benefit from a higher spatial resolution perpendicular to the incident electron beam (see Section 1). In addition to the local lattice orientation, OIM measures the quality of the EBSD pattern at each point of the grid. The shades of grey in Fig. 5.8a scale with the pattern quality from the region shown in Fig. 5.5: darker spots represent EBSD patterns of poorer quality and black spots correspond to non-indexed patterns. Characteristic dark stains in the OIM are possibly produced by precipitates. In Fig. 5.8b, bold lines indicate misorientations higher than 15° and thin lines refer to misorientations in the range, 1.5°-15°. It is seen that the pattern quality index is high within grain fragments and low at their boundaries. The spacing between resolved dislocation boundaries is \(\sim2\mu\)m.

Comparing these orientation maps with the images collected in the TEM, it is evident that the SEM/OIM technique incompletely reveals the CB subdivision pattern. Banded structures are observed in many grains, but subdivision on a finer scale is frequently not resolved. Individual cells visible in the TEM are only occasionally revealed by OIM (Fig. 5.5). Nevertheless, some important characteristics of the CB structure described in Chapter 2 are also observed here: grains are subdivided by one or two families of extended planar dislocation boundaries that show a macroscopic directionality (+ and/or - 40° to
Fig. 5.4 Orientation map obtained on the 40% cold rolled aluminium. Three grains are highlighted for detailed analysis in Fig. 5.10.
Fig. 5.5 Orientation map showing a close-up on a strongly subdivided grain from Fig. 5.4. (EB is the direction of the incident electron beam.)
Fig. 5.6 Orientation map from the 40% cold rolled aluminium (RD is vertical). On the right, the shading is proportional to the misorientation $\theta_M$ relative to the grain *mean orientation*. 
Fig. 5.7 Orientation map from the 40% cold rolled aluminium.
RD), the thickness of the cell blocks in-between is ~2µm, and the misorientation across the CB boundary ranges from ~1° to ~15°. It is also noteworthy that these extended planar dislocation walls sometimes appear to originate from steps (or irregularities) in the grain boundary (Fig. 5.6 and Fig.
5.7). Supplementary to the CB pattern, OIM clearly identifies a large-scale subdivision which will be characterised in the subsequent section.

Finally, one may try to assess whether the spatial resolution or the angular accuracy of OIM is more critical for the examination of such deformation structure. The present OIM observations tend to indicate that the spatial resolution is not so critical. (i) No difference of sharpness is seen between the horizontal and the vertical direction in the scans whereas the diffracting volume is elongated ~3 times in the latter direction (see Section 1). (ii) According to the “image quality” map (Fig. 5.8a), corresponding to the close-up on the highly subdivided grain (Fig. 5.5), the diffraction pattern arising from within cell blocks had a much better contrast than the pattern produced when crossing CB boundaries. (iii) The scans performed on the high-resolution FEG microscope did not generate nicer maps (1). On the other hand, from the comparison with the previous TEM results, it appears that many CBs were not identified by OIM. This is probably due to the fact that the misorientation across these CB walls was lower than the angular accuracy of OIM.

2.3.2 Illustration of the heterogeneity of subdivision

From the colour variations in the orientation maps, one can tell that grains undergo different types and/or levels of subdivision. This heterogeneity is also revealed if the local orientations measured within each grain are presented in separate pole figures. This has been carried out for six grains of the orientation map shown in Fig. 5.7.

- Grains #1 is clearly subdivided into CBs and its pole figure reveals a significant orientation range.
- No CBs are seen in Grain #2. Therefore, the orientation spread in the pole figure must be due to long-range gradients. Note that the mean orientation of this grain is cube \{001\}<100>.
- Grain #3 has a large mapped area but the markings in the pole figure are smaller than the previous ones. This is a sign of low orientation gradients (if any).

(1) The spatial resolution obtained with the W-filament microscope was confirmed to be 0.3-0.5µm when scanning two other aluminium grades with a much smaller grain size (~1µm). This was done in collaboration with Saimoto et al (2000) and with E. Rauch.
• Grain #4 contains two families of CBs. The orientation spread shown by the pole figure is important, and it is more “isotropic” than for Grain #1.

• The analysis made for Grain #3 also applies to Grain #5.

• Grains #6 contains CBs but their relative misorientations must be low, as revealed by the small markings in the pole figure. (Note that this grain was mapped on a larger area than what is shown in Fig. 5.7.)

Fig. 5.9 Illustration of the subdivision heterogeneity by plotting <100> pole-figures separately for various grains mapped in Fig. 5.7. The light spot in the centre of the markings indicates the grain mean orientation calculated with the procedure presented in Section 3.1. (RD is the horizontal axis and TD the vertical one.)

The subdivision heterogeneity is also revealed by analysing the evolution of lattice orientation along parallel lines in a map. Three segments parallel to RD are defined in the orientation map shown in Fig. 5.4. The black line in Fig. 5.10a-c represents the evolution of $\theta_M$ along the three analysed segments, where $\theta_M$ denotes the misorientation of each grid-point relative to the grain.
mean orientation \(^{(1)}\). The grey line in Fig. 5.10a-c indicates the value of the relative misorientation \(\theta_{rel}\) between successive grid-points. The misorientation distributions in Fig. 5.10a-c provide useful information about the microstructure of the sampled grains.

\[ \theta_{rel} \]

Fig. 5.10 Illustration of the heterogeneity of subdivision by analysing local orientations across 3 characteristic grains.

- Grain #1 has developed a well-defined cell block structure, where sharp boundaries delineate fragments with alternating lattice orientations (see also Fig. 5.5 and Fig. 5.8). This yields relatively large \(\theta_{rel}\) values at regular intervals along the segment and \(\theta\) ranging between 5\(^{\circ}\) and 15\(^{\circ}\).

\(^{(1)}\) To be defined in the next section.
The orientation spread within grain #2 is smaller. $\theta_{rel}$ mostly remains below 3° and $\theta_M$ approaches 10° only in a few locations.

In grain #3, $\theta_M$ reaches values beyond 15°, although $\theta_{rel}$ remains low (typically less than 3°). The orientation seems to change continuously over distances of 10-20µm along RD.

This comparison illustrates that the orientation spread within a plastically deforming grain may have different origins. In some grains (e.g. grain #1), the orientation spread is created by dislocation boundaries accommodating large misorientations. Other grains (e.g. grain #3) contain “long-range” (10-20µm) orientation gradients, which bear some similarity with the gradients predicted in finite element studies relying on an accurate reproduction of the microstructure (Becker and Panchanadeeswaran, 1995; Mika and Dawson, 1999; Delaire et al, 2000; Bhattacharyya, in press). It is possible that TEM would reveal a fragmentation of such grains into cells or cell-blocks having small cumulative misorientations. However, this is not visible in the present orientation maps due to the limited resolution of the SEM/EBSD technique.

The misorientation line-plots demonstrate that both the “long-range” orientation gradients and the fragmentation into CBs can create large orientation spreads relative to the grain mean orientation, i.e. to $\theta_M$ values larger than 15°. However, the fragmentation into CBs yields larger $\theta_{rel}$ values on average.

### 3 Statistical analysis of grain subdivision from the OIM data

In this section, a computational procedure is proposed for characterising the orientation spreads revealed in individual grains. The procedure has been applied to 16 orientation maps, including the maps shown in Figs.4, 6 and 7. The purpose was to determine whether a correlation exists between the mean orientation of a grain and the type and/or level of subdivision that is revealed by OIM. Here, the orientation spread will not be qualitatively characterised (like in the previous section), but quantitatively. The results should later be used for validating simulations by various plasticity models (Chapter 6).
3.1 Reconstruction of grains

3.1.1 Limitations of the traditional method

The first step in the orientation map analysis is the identification of original grain boundaries. The traditional way to do this strictly relies on the calculation of misorientations between immediate neighbours in the OIM grid. Frequently, it is assumed that two neighbours with a misorientation of less than 15° belong to the same grain.

Such a procedure is efficient when applied to recrystallised materials, but is less reliable in deformed microstructures where subgrain boundaries with fairly large misorientations can be produced by subdivision (e.g. Liu et al, 1998a). Also, no misorientation can be computed at OIM grid points where pattern indexing was not successful, which is often the case for subgrain boundaries (see Fig. 5.8). To overcome this, the traditional recognition method requires a careful preliminary clean-up of the data that removes “zero solutions” (Wright, 1993).

In view of these limitations, a new grain recognition approach was developed for materials deformed to low and moderate strain levels. Before this new approach is presented, the concept of mean orientation should be introduced.

3.1.2 Definition of a “mean orientation” – Use of quaternions

The mean orientation in a set of discrete orientations is here defined as the lattice orientation that has the minimum misorientation to all orientations constituting the set. It is computed most easily when lattice orientations are expressed as quaternions (Altmann, 1986):

\[ q_0 = \cos \left( \frac{\Psi}{2} \right) \quad \text{and} \quad q_j = n_j \sin \left( \frac{\Psi}{2} \right) \quad j = 1..3 \]  

(1)

where \( n_j \) and \( \Psi \) designate, respectively, the axis and the angle of the rotation bringing the sample reference axes on the crystal axes corresponding to the given orientation. The misorientation \( \theta_{M,k} \) between the crystal orientation represented by \( q_j^k \) and the (yet unknown) grain mean orientation \( q_j^M \) can be expressed as

\[ \theta_{M,k} = 2 \cos \left( \frac{1}{2} \left( | q_0^k q_0^M + q_1^k q_1^M + q_2^k q_2^M + q_3^k q_3^M | \right) \right). \]  

(2)
By definition, the co-ordinates \( q_j^M \) of the quaternion representing the \textit{mean orientation} must be such that they minimise the average misorientation \( \theta_{M,k} \) where \( k \) covers all orientations in the set. In practice, we rather maximise

\[
\sum_k \left( \sum_{j=0,4} q_j^M q_j^k \right) = \sum_k \cos \left( \theta_k^M / 2 \right) = \text{Max}
\]

under the constraint that

\[
\sum_{j=0,4} \left( q_j^M \right)^2 = 1.
\]

The latter is a property of all quaternions (see Eq.1). The convergence of this constrained maximisation is very fast if one uses, as first estimate of \( q_j^M \), the arithmetic average of all \( q_j^k \).

Of course, one must also pay attention that each lattice orientation has 24 equivalents due to the symmetry of cubic lattices (Chapter 1). The 24 sets of co-ordinates \( q_j^k \) representing the symmetrical equivalents of the \( k \)th orientation can be derived using quaternions (Van Acker, 1996). After the first maximisation of Eq.3, it is checked that the co-ordinates \( q_j^k \), which have been used, represent well the symmetrical equivalent that is closest to \( q_j^M \) (i.e. that yields the smallest \( \theta_{M,k} \) value). If this is not the case, the maximisation is performed a second time using new \( q_j^k \) co-ordinates.

Finally, it should be noted that \( \theta_{M,k} \) was denoted \( \theta_M \) in Fig. 5.10 and that quaternions are also used for computing the misorientation \( \theta_{rel} \) between adjacent points of the OIM grid.

\textbf{3.1.3 New grain recognition procedure}

Now that the concept of \textit{mean orientation} has been introduced, the new procedure for identifying original grain boundaries can be presented. It consists of the following three steps:

- To start, the standard method for grain recognition (section 3.1.1) is applied with a small tolerance angle (3° instead of 15°). This yields a series of subsets that correspond to fragments of the original grains.
- Fragments of the same parent grain are subsequently assembled in an iterative procedure. For this, the \textit{mean orientation} of each subset is
determined and the misorientation between the mean orientations of any pair of adjacent fragments is also computed.

- Then, the two adjacent fragments with the smallest misorientation are assembled into a larger subset (having a new mean orientation).

This last step is repeated iteratively until the minimum misorientation between the remaining adjacent fragments becomes larger than 10°. For larger misorientations, the analysis is refined and requires the operator’s intervention: adjacent fragments with misorientations up to 20° are assembled only if they form banded structures with alternating lattice orientations. This refinement approach is based on existing TEM observations of deformation structures in aluminium cold rolled to a similar strain (e.g. Bay et al, 1992).

3.1.4 Recognition of original grain boundaries in the 16 orientation maps

Applying the new grain identification procedure to the 16 orientation maps recorded in the aluminium plate, more than 450 original grains could be reconstructed. Some of these grains had a very small mapped area because the grain lay on the edge of a scan, or because the grain was sectioned at its edge. If the mapped area is too small compared to the grain size, it does not provide reliable information about the subdivision of the corresponding grain. Indeed, areas close to triple junctions and grain boundaries may demonstrate a modified deformation pattern. The analysis was, therefore, restricted to the 352 grains having each a mapped area larger than 500µm².

The 352 grains stem from 16 different locations in the bulk of a deformed plate, i.e. the 16 orientation maps. These grains have unknown original orientations but their mean orientations after rolling can be computed during grain reconstruction. The ODF shown in Fig. 5.11 was constructed by superimposing spherical gaussian-distributions on the 352 mean orientations (Bunge, 1982; Van Houtte, 1995). The gaussians had a half-scatter width of 7° and a weight proportional to the mapped grain area. By comparing Fig. 5.11 to the ODF derived from pole figure measurements on the same material (Fig.10 in Chapter 4), one may check that the orientations of the 352 grains are statistically representative of the macroscopic texture. Only the proportion of grains with the brass orientation \{110\}<112> is too high in the OIM sampling. Considering that the plates have a significant through-thickness texture gradient (Mishin et al, 2000) and that the orientation maps were recorded at different depths, the reproduction of the macroscopic texture is satisfactory.
3.2 Characterisation of grain subdivision

Based on the observation of Fig. 5.10a-c, it is proposed to characterise grain subdivision by averaging the parameters $\theta_M$ and $\theta_{rel}$ over the area of each reconstructed grain. The averaged values $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ were computed for the 352 mapped grains. In grains subdividing into highly misoriented fragments like grain #1 (of Fig. 5.10), high values of both $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ were obtained. Conversely, grains that subdivided to a smaller extent (like grain #2) produced low values of $\bar{\theta}_M$ and $\bar{\theta}_{rel}$. Grains similar to grain #3, i.e. containing “long-range” (10-20µm) orientation gradients but low misorientations between adjacent fragments, had a high $\bar{\theta}_M$ and a low $\bar{\theta}_{rel}$. In general, the largest $\theta_M$ values were found in the vicinity of grain boundaries and triple junctions (lighter regions in Fig. 5.6b). Table 1 presents the mean orientations of the three grains highlighted in Fig. 5.4 along with their $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ values.

In designing the parameters, it was hoped that $\bar{\theta}_{rel}$ would estimate the average misorientation between cell blocks. However, as the OIM step-size is sometimes smaller than the average cell size, more than one measurement is susceptible to be made within each cell, thus reducing $\bar{\theta}_{rel}$. Furthermore, any relative misorientation lower than the angular accuracy of EBSD measurements (1-2°) is counted as a zero misorientation. This problem is eliminated by introducing a complementary parameter $\bar{\theta}_{CB}$ which is calculated similarly to $\bar{\theta}_{rel}$ except that it only includes relative misorientations larger than 2°. The $\bar{\theta}_{CB}$ value that is obtained for the grains highlighted in Fig. 5.4 is given in Table 1.

\begin{itemize}
\item For determining $\bar{\theta}_{rel}$ relative misorientations $\theta_{rel}$ were measured in the six directions of a hexagonal grid.
\end{itemize}
Table 1 Characteristics of orientation spreads within the three grains selected in Fig. 5.4

<table>
<thead>
<tr>
<th>Miller Indices</th>
<th>Mapped Grain Area</th>
<th>Misorientations (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>{ h k l }</td>
<td>&lt; u v w &gt;</td>
<td>( \bar{\theta}_M )</td>
</tr>
<tr>
<td>1</td>
<td>0.86 -0.51 0.11</td>
<td>-0.49 -0.86 -0.16</td>
</tr>
<tr>
<td>2</td>
<td>0.69 0.72 0.07</td>
<td>0.51 -0.55 0.66</td>
</tr>
<tr>
<td>3</td>
<td>-0.99 0.09 0.12</td>
<td>-0.09 -0.99 0.03</td>
</tr>
</tbody>
</table>

Finally, the question whether the value of \( \bar{\theta}_M \) depends on the area of the sampled grains has been considered. For grains developing “long range” orientation gradients (like grain #3), it is expected that \( \bar{\theta}_M \) increases with increasing grain area. Indeed, as \( \bar{\theta}_{rel} \) is low in these grains, building up large misorientations relative to the grain mean orientation is only possible over large distances. On the other hand, the \( \bar{\theta}_M \) value of grains subdividing into fragments with alternating misorientations (like grain #1) should be almost independent of the grain area. Analysing \( \bar{\theta}_M \) values obtained in the sixteen OIM scans, it appears that the grain area effect on \( \bar{\theta}_M \) is different for grains with different orientations. In Fig. 5.12, the \( \bar{\theta}_M \) value is plotted against the equivalent grain-area diameter: \( D = (\text{Grain Area})^{1/2} \). In grains with cube \{001\}<100> and rotated cube \{025\}<100> and \{205\}<502> orientations, the \( \bar{\theta}_M \) values tend to increase with increasing grain area, whereas the \( \bar{\theta}_M \) values for the S \{123\}<634> and copper \{112\}<111> components seem to be independent of the grain area. Grains with the brass \{110\}<112> orientation show ambiguous behaviour: both very large and very low \( \bar{\theta}_M \) values are found whatever the grain area.

It thus appears necessary to correct \( \bar{\theta}_M \) for the grain area effect. This is done based on an analysis of the average trend among the 352 grains. On average, the \( \bar{\theta}_M \) value of the 352 mapped grains was found to increase by 0.25° when the equivalent grain-area diameter \( D \) increases by 10\( \mu \)m. A fourth parameter was defined by correcting empirically \( \bar{\theta}_M^C \) for this grain-area effect:

\[
\bar{\theta}_M^C = \bar{\theta}_M - 0.25° \cdot \left( \frac{\text{Grain Area}^{0.5}}{10\mu m} \right)
\]  

(3)
3.3 Lattice orientation effect on grain subdivision

In order to check whether a correlation exists between the mean orientation of a grain and the orientation spread resulting from subdivision, ODFs were generated separately for grains having either high or low $\bar{\Theta}_M$, $\bar{\Theta}_C$, $\bar{\Theta}_{rel}$ or $\bar{\Theta}_{CB}$ values (Figs. 5.13 - 5.16). In these ODFs, all selected grains were assigned the same weight independent of their area. Two ODFs representing the orientations of grains having the 125 highest and the 125 lowest $\bar{\Theta}_M$ values are shown in Fig. 5.13. The intensity of the cube and rotated cube components is 2-5 times larger in the “high-$\bar{\Theta}_M$” ODF (Fig. 5.13a) than in the “low-$\bar{\Theta}_M$” ODF (Fig. 5.13b). The opposite trend is found for orientations along the $\beta$-fibre. In Fig. 5.14a-b, grains are selected based on their $\bar{\Theta}_{rel}$ values, demonstrating that the orientation effect revealed by Fig. 5.13 cannot be attributed to a grain-area effect alone. In Fig. 5.15, the two ODFs represent grains with either the 125 highest or the 125 lowest $\bar{\Theta}_{rel}$ values. The cube, RD-rotated cube and brass orientations have high intensities in the “low-$\bar{\Theta}_{rel}$” ODF, whereas the TD-rotated cube intensity is largest in the “high-$\bar{\Theta}_{rel}$” ODF (Fig. 5.15a). The same tendency is found in Fig. 5.16, where grains are selected according to their $\bar{\Theta}_{CB}$ value.
Fig. 5.13  ODFs generated by superposing gaussian distributions on the orientations of grains with a) the 125 largest $\theta_M$ values, b) the 125 lowest $\theta_M$ values. Contour lines: 1.0, 2.5, 5.0.

Fig. 5.14  ODFs generated by superposing gaussian distributions on the orientations of grains with a) the 125 largest $\theta_M^C$ values, b) the 125 lowest $\theta_M^C$ values. Contour lines: 1.0, 2.5, 5.0.
Chapter 5  Statistical study of the heterogeneity of subdivision

Fig. 5.15  ODFs generated by superposing gaussian distributions on the orientations of grains with a) the 125 largest $\theta_{\text{rel}}$ values, b) the 125 lowest $\theta_{\text{rel}}$ values. Contour lines: 1.0, 2.5, 5.0.

Fig. 5.16  ODFs generated by superposing gaussian distributions on the orientations of grains with a) the 125 largest $\theta_{\text{CB}}$ values, b) the 125 lowest $\theta_{\text{CB}}$ values. Contour lines: 1.0, 2.5, 5.0.
These orientation effects are also established by specifically analysing the parameter values calculated in grains having one of the six particular orientations represented in Fig. 4.3 (cube, RD-rotated cube, TD-rotated cube, brass, S and copper). Out of the 352 mapped grains, 235 had a mean orientation within 15° of one of the six orientations. The $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ values of the 235 grains with typical orientations are plotted in Fig. 5.17, also indicating their mean and their standard deviation. It is seen that there is a considerable spread in both the $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ values. However, grains with near-cube orientations are usually characterised by larger $\bar{\theta}_M$ values compared to grains having orientations along the $\beta$-fibre. Also, the $\bar{\theta}_{rel}$ value is larger for the TD-rotated cube and copper orientations and somewhat smaller for the cube, RD-rotated cube and brass orientations. The same type of spread is found for the $\bar{\theta}_M$ and $\bar{\theta}_{CB}$ parameters.

The $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ values of the remaining 117 grains that were oriented close to none of the characteristic orientations are also plotted in Fig. 5.17. These grains are represented by the label “Other” and are characterised by high $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ values on average. They constitute the “random background” of the ODFs shown in Fig. 5.13-16.

4 Discussion

The procedure proposed for analysing orientation maps allows a systematic and automatic recognition of grains with distinct subdivision progress. The parameters $\bar{\theta}_M$ and $\bar{\theta}_C$ measure the overall orientation spread that has developed within each grain during deformation. Using the parameters $\bar{\theta}_{rel}$ or $\bar{\theta}_{CB}$, it is also possible to distinguish between grains containing “long range” (10-20µm) orientation gradients and grains forming small fragments with large misorientations.

It is clear that the characterisation of subdivision would have been more precise if one would have used the TEM to analyse each grain separately, manually selecting fragments for orientation indexing and applying elaborated rules to derive long range orientation gradients in prescribed directions (Pantleon, 2000). It is then an immense task to gather statistically reliable information over a large number of grains.
Fig. 5.17 $\bar{\theta}_M$ and $\bar{\theta}_{rel}$ values of the 235 grains oriented within 15° of a characteristic texture components (cube, RD-rotated cube, TD-rotated cube, brass, S or copper) and of the 117 “other” grains. The average and the standard deviation are also indicated.
The observations made here on 352 grains from 16 orientation maps are in agreement with previously reported TEM findings. In addition, OIM observations provide some new insight about long-range subdivision mechanisms.

The 125 grains with the largest $\theta_M$ and $\theta_C$ values, i.e. grains containing large misorientations relative to the grain mean orientation, have lattice orientations mostly in the vicinity of the cube $\{001\}<100>$ and rotated cube ($\{025\}<100>$ and $\{205\}<502>$) components. Among these grains, those with orientations closer to the cube and the RD-rotated cube orientations have low $\theta_{rel}$ values, suggesting that orientation spreads arise from long-range orientation gradients. This result is consistent with the well-known finding of Dillamore and Katoh (1974), who demonstrated that near-cube orientations form important lattice curvatures during rolling because they lie in a “divergent” region of Euler space. Several regions of the grain rotate towards distinct stable texture components, but the grain centre maintains a cube orientation throughout deformation. (see Chapter 2).

In grains with the TD-rotated cube $\{205\}<502>$ orientation, both the $\theta_M$ (or $\theta_C$) and the $\theta_{rel}$ (or $\theta_{CB}$) values are higher than the average. This indicates a tendency to form fragments with high misorientations (e.g. Fig. 5.5). Note that high misorientations across cell-block boundaries in grains with orientations close to $\{001\}<100>$ have also been found in a TEM analysis of a similar material (Liu et al, 1998a). In that study, however, the nearby RD-rotated cube and TD-rotated cube components were not considered specifically. In another cold-rolling experiment, a single crystal of cube orientation has been reported to subdivide into so-called “deformation bands” having mirror $\{205\}<502>$ orientations, which were separated by “transition bands” with the $\{001\}<100>$ orientation (Liu and Hansen, 1998). The former bands were subdivided into cell blocks with alternating misorientations whereas the transition bands contained equiaxed cells with cumulative misorientations. The appearance of bands with $\{205\}<502>$ orientation was attributed to RD-ND shear on top of the plane strain compression. The formation of cell-blocks within them was explained by slip imbalance among the most stressed slip systems (Liu and Hansen, 1998).

The subdivision patterns observed in the single crystal concord with the present results. Here, the RD-ND shear within grains of $\sim\{205\}<502>$ orientation might, however, be due to interactions with the neighbouring grains rather than friction with the rolls as in the single crystal experiment.
The OIM study has shown that the orientation spread is less prominent in grains with β-fibre orientations than in grains with cube and rotated cube orientations. This is revealed by lower $\bar{M}_M$ (and $\bar{C}_M$) values. Also, the brass orientation is associated with slightly larger $\bar{M}_M$ (and $\bar{C}_M$) values than the S and copper orientations, whereas the $\bar{\theta}_{rel}$ values increased from the brass to the copper orientation. The latter result is consistent with several channel-die compression studies, where single crystals having the brass $\{110\}<112>$ orientation showed rather homogeneous subdivision structures with low in-grain misorientations compared to single crystals of the S and copper orientations (Driver et al, 1994; Godfrey et al, 1998a,b). In addition, our experiment shows large $\bar{M}_M$ values in some grains oriented close to the brass component, which indicates a tendency to form long-range orientation gradients. The reason why this has not been observed in the previous channel-die experiments (Driver et al, 1994) may be the lack of constraint against RD-TD and RD-ND shears when a sample is compressed in a channel-die. Under this condition, brass oriented single crystals have been reported to undergo severe RD-TD shear (Aernoudt and Stüwe, 1970; Driver et al, 1994). In a polycrystal, however, RD-TD shears are constrained by the neighbouring grains. Thus, the opportunity for a brass oriented grain to shear under RD-TD, strongly depends on the orientation of the adjacent grains. Such interactions may result in a heterogeneous strain within brass oriented grains, which would contribute to the long-range orientation gradients revealed by OIM.

Another result of the OIM study is that grains oriented close neither to the cube component nor to the β-fibre have higher $\bar{M}_M$ and $\bar{\theta}_{rel}$ values than the average (Fig. 5.17). This concords with the observations made by Fortunier and Driver (1987) on 24 coarse grains in a polycrystalline aluminium sample. The largest orientation spreads were found in grains that did not rotate towards any stable texture component.

Besides the orientation effects described above, there was an important scatter in both the $\bar{M}_M$ (or $\bar{C}_M$) and the $\bar{\theta}_{rel}$ (or $\bar{\theta}_{CB}$) values. This scatter may be attributed to the fact that the deformation of a grain is not solely dependent on the current lattice orientation. It also likely depends on the grain shape and size, on the presence of precipitates and on the orientation and the topology of neighbouring grains. Also, grains having a similar lattice orientation after 40% rolling may actually have totally different deformation histories, especially if their initial orientations are different. Considering all of this, the fact that one
can still observe a correlation between the mean orientation and the type/level of subdivision is remarkable.

From the extent of the orientation gradients and fragment misorientations observed in this study and in the related TEM work, one may reasonably expect that introducing grain subdivision mechanisms in texture prediction models would significantly improve their performances. In this regard, the experimentally observed orientation effects on subdivision are particularly interesting. It is evident that new polycrystal plasticity models accounting for grain subdivision should be judged not only on the macroscopic texture prediction, but also on their ability to reproduce correlations between the local orientation and the type/level of subdivision.
CHAPTER 6: PREDICTING GRAIN SUBDIVISION USING THE LAMEL MODEL AND A FE MODEL

In Chapter 4, it has been demonstrated that models taking grain interactions into consideration yield improved prediction of macroscopic rolling textures in steel and aluminium. This was true for the LAMEL model that considers idealised interactions between each grain and only one of its neighbours, as well as for the FE model allowing a large variety of interactions with many neighbours. Although the FE model required much more computing time than the LAMEL model did, its texture predictions were only slightly better in aluminium, and not better in steel (1).

The OIM observations in Chapter 5 have shown that the deformation microstructure in cold rolled aluminium is very heterogeneous. Some grains develop long-range orientation spreads whereas others are split into small fragments with large misorientations. The statistical analysis revealed significant orientation effects on subdivision, which constitutes valuable information for testing plasticity models at the scale of individual grains.

As we will see in the present chapter, both the LAMEL model and the FE model can simulate the development of intra-granular orientation gradients. The assumptions made by either models are, however, quite different and the predicted intra-granular orientation gradients are different too. One hypothesis that the two models do have in common is that in-grain heterogeneities are triggered solely by the interaction with neighbouring grains. Therefore, the grains that are expected to split most are the grains that are most sensitive to grain interactions, i.e. grains in which strain and stresses are significantly influenced by the surrounding.

(1) In steel, the original LAMEL model led to the best texture predictions, but in aluminium, it was necessary to add a supplementary relaxation to the original LAMEL model: the RD-TD shear.
Supplementary to this, it will be shown that the LAMEL model can be adapted so that it considers interactions among subgrains, instead of grain interactions. This permits a study of the increasing misorientation between adjacent cell blocks or deformation bands. Here, grain subdivision is assumed to be solely dependent on the grain orientation. It is independent of the surrounding.

1 Modelling the effect of grain interactions on the formation of “long-range” orientation gradients

In this section, an attempt is made to reproduce the long-range orientation gradients that have been revealed by OIM in Chapter 5. We will check whether the right orientation effects on subdivision can be predicted if we assume that the formation of such gradients is driven solely by grain interactions. By applying either the FE model or the LAMEL model, we will distinguish between two situations. In the first case, the slip activity varies constantly and uniformly from one edge of the grain to the other, whereas in the second situation grains are split into regions that interact preferentially (and even exclusively!) with the closest neighbouring grain.

The 10-20µm wide orientation gradients observed by OIM cannot be classified a priori as one of these two extreme situations. The micromechanical function of the experimentally observed gradients is somewhere in-between. One way to assess whether one situation is more correct is to check whether one assumption allows better reproducing the correlation found between the grain mean orientation and the in-grain orientation spread.

1.1 FE simulations

“Grain scale” FE models (Chapter 3) partition stresses and strains over the polycrystal by enforcing stress equilibrium and strain compatibility along all grain boundaries. The predicted dislocation slip activity is thus non-uniform within each grain, leading to non-uniform lattice rotations and to the development of intra-granular orientation gradients. The latter depend obviously on the shape, the orientations and the topology of the interacting grains. In order to determine whether some grain orientations tend to form larger orientation
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gradients upon deformation, one has to study how a grain having this orientation behaves, on average, in a variety of neighbourhoods.\(^{(1)}\)

The information about the microstructure studied by OIM is only two-dimensional and it concerns only the final deformation state (i.e. the initial grain orientations are unknown). Therefore, FE modelling can hardly be used to reproduce the exact same deformation microstructure. Instead, the choice is here made to perform the FE simulations on a model microstructure in which all grains have the same shape and in which the initial orientations are generated by discretising the macroscopic texture.

The FE simulations carried out in this chapter are very similar to those performed in Chapter 4, where the aim was to predict the macroscopic texture evolution. We make use of the same mesh containing 10(RD)x12(TD)x10(ND) = 1200 elements (see Fig. 4.4). As each grain is represented by a single 8-noded cubic element, the strain, the stress and the slip rates change linearly in whichever direction across the grain (Chapter 3). It is clear that such simulation is an oversimplification of reality, and that more realistic predictions should be obtained if the mesh was finer (~100 elements per grain), and if the grain arrangement was less regular. Nevertheless, representing each grain with a single element is interesting from a fundamental viewpoint because it is complementary to another idealised situation that is to be simulated later with the LAMEL model.

We are now interested in the evolution of grains having characteristic initial orientations and, more precisely, in the creation of an orientation spread within these grains. The predicted in-grain orientation spread is characterised at the end of the simulation in the following way:

- First, the mean orientation of each grain is calculated by averaging the orientations predicted at the 8 nodes constituting the grain. (For this, quaternions are used as already suggested in Chapter 5.)
- Then, we compute the average misorientation between the grain mean orientation and the orientations predicted at the 8 nodes.

\(^{(1)}\) Note that this was also true in the OIM analysis performed in Chapter 5. We have studied how grains with e.g. the cube orientation behaved on average in the 16 orientation maps.
Supplementary to this in-grain orientation spread, the simulation provides useful information about the history of deformation. The initial orientation of each grain is known, which enables computing the misorientation between the initial orientation and the final mean orientation of the grain. One may also analyse to what extent two grains, which had initially the same orientation but a different location in the mesh (thus a different neighbourhood), rotate apart of one another. For this, we compute the misorientation between the final mean orientation of the two grains. Even though there are no experimental measurements for validating these results \(^{(1)}\), it is interesting to compare such inter-granular misorientations to the misorientations predicted to arise inside individual grains.

1.1.1 First type of FE simulations: 24 grains imbedded in a matrix

A first set of FE simulations was designed to investigate the deformation of 24 grains bearing a common initial orientation. These grains were distributed in the mesh interior so as to avoid direct interactions among them. This is illustrated in Fig. 6.1 showing six consecutive sections of the mesh that contain 14 of the 24 grains. The orientation assigned to the 24 grains was one of the six characteristic orientations used in the OIM study (cube, RD-rotated cube, TD-rotated cube, brass, S, copper). The orientations of the other 1176 “matrix” grains were representative of a random texture, which ensures that the 24 grains have very distinct neighbourhoods.

Six simulations were carried out, with as only difference from one simulation to the next, the orientation assigned to the 24 grains. The effect of this initial orientation on the orientation spread developing within the 24 grains was evaluated after 15% and 40% rolling reduction. The values obtained from the six simulations are presented in Fig. 6.2. Besides the intra-granular orientation spread, Fig. 6.2 shows the average misorientation between the initial orientation of the 24 grains and the 24 mean orientations after deformation. Furthermore, the inter-granular orientation range was computed as the average misorientation between any two of the 24 mean orientations after deformation. (This means the average of 24*(24-1)/2=276 misorientations.)

\(^{(1)}\) We have seen in Chapter 2 that it is impossible to record, by a non-destructive experimental technique, the deformation of any specific grain imbedded in the bulk of a polycrystal.
The results presented in Fig. 6.2 can be interpreted as follows:

- The *intra-granular orientation spread* (measured by the average misorientation of the 8 nodes relative to the grain *mean orientation*) becomes significantly different for the six characteristic orientations, only after 40% rolling. The largest value is obtained for *TD-rotated cube* and the lowest ones correspond to the β-fibre orientations.

- Whichever the initial orientation of the 24 grains, the *inter-granular orientation spread* (the average misorientation between any two of the 24 grains) is at least twice larger than the corresponding average *intra-granular orientation spread*.

- The average misorientation relative to the initial orientation is also larger than the *intra-granular orientation spread*. Note that, for the matrix grains, this value is ~13° (after 40% rolling). This is thus larger than the values obtained for the 24 grains, demonstrating that the six characteristic orientations are relatively stable with respect to texture evolution.
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Intra-granular orientation spread (avg miso of the 8 nodes relative to the grain mean orientation)

Avg miso between the final grain orientation and the initial orientation

Inter-granular orientation spread (avg miso between any two of the 24 final mean orientations)

Fig. 6.2 Orientation range developing within 24 grains that have a common initial orientation (indicated in the graphs) and are imbedded in a matrix bearing a random texture.
Another set of six simulations was conducted with matrix grains that were representative of a rolling texture (the AA3104 cold-rolled 70%, Fig. 4.14) instead of a random texture. It was checked that the texture of the matrix grains has a marginal effect on the average orientation spreads in the 24 grains with characteristic orientations.

1.1.2 Second type of FE simulation: different spatial arrangements of the same set of 1200 grains

There is a clear difference between the previous simulations and the OIM experiment: in the simulations, the grains have characteristic initial orientations, whereas the correlation revealed by the OIM analysis concerns the final grain orientations. As the $\beta$-fibre was absent from the initial experimental texture (the undeformed AA1050 texture consisted of a weak cube component), it is not likely that grains oriented along the $\beta$-fibre after 40% cold rolling had such orientations already from the start. Therefore, it might be more correct to use the texture measured in the undeformed AA1050 plate as input for the FE simulation, and to study orientation effects on subdivision based on the mean orientations predicted after 40% rolling (instead of the initial orientations).

However, as we mentioned previously, it is not sufficient that a grain develops a large orientation spread during one such simulation, to justify the conclusion that this grain has a strong tendency to subdivide. In order to draw correct conclusions, the same grain must be considered in a variety of neighbourhoods. We have therefore performed 8 simulations of 40% cold rolling, relying on the same FE mesh of 1200 cubic elements as in the previous section. The same 1200 initial orientations were used in the 8 simulations, but each orientation was assigned to a different finite element from one simulation to the other. Applying a tracking procedure, we have compared the deformations that each grain underwent in its 8 distinct neighbourhoods (i.e. in the 8 simulations).

In order to study the correlation between the mean orientation of the grain and the intra-granular orientation spread, we have investigated specifically the grains that were found to be oriented within 15° of one of the six characteristic orientations after 40% rolling. Similarly to the previous section, three types of misorientation were computed: (i) the average misorientation between the 8 nodes and the mean orientation of each grain (intra-granular orientation spread), (ii) the misorientation of the final mean orientation with respect to the
initial orientation, and (iii) the average misorientation between any 2 of the 8 final grain orientations that were predicted during the 8 simulations (and correspond to 8 different surroundings of the grain). A summary of the results in presented in Fig. 6.3.

![Graph showing orientation spread](image)

**Fig. 6.3** Summary of the 8 rolling simulations performed on different spatial arrangements of 1200 grains that represent initially the texture of the undeformed AA1050 plate.

The following conclusions can be drawn about the results shown in Fig. 6.3:

- The correlation observed between the mean orientation of the grains and the *intra-granular orientation spread* is the same as in the previous section. The average orientation spreads are larger for grains oriented near *cube* than for those oriented along the β-fibre.
• As expected, grains oriented along the $\beta$-fibre after 40% rolling did not have such orientations initially. This is confirmed by the large average misorientation relative to their initial orientations.

• The final orientation of a grain is strongly dependent on the grain surrounding (i.e. it varies very much from one simulation to the other). The inter-granular orientation range is $\sim$ twice larger than the intra-granular orientation range.

• It is noteworthy that grains oriented close to none of the six characteristic orientations yield very large orientation spreads (these grains are represented by the label “Other” in Fig. 6.3).

This last conclusion concerning the 493 (out of 1200) grains that did not rotate towards a characteristic orientation is in agreement with the OIM findings. In Fig. 6.4, the accumulated probability function is given for the three types of misorientation. It shows, for example, that the average misorientation between the 8 nodes and the grain mean orientation is less than 7° in 80% of all grains.

![Misorientation Distribution](image)

**Fig. 6.4** Accumulated probability function showing the proportion of grains for which the intra- or inter-granular orientation spread or the average misorientation relative to the initial orientation is less than $x^\circ$. 
1.2 Simulations using the LAMEL model

The simulations performed in the previous section, using FE modelling, have provided a first prediction of the orientation gradients developing within the grains. These simulations relied on a simplifying assumption stating that the lattice orientation varies constantly from one edge of the grain to another.

We now consider another idealised situation, in which the interaction with adjacent grains is still the unique origin of intra-granular heterogeneity. In this new situation, illustrated in Fig. 6.5a, it is assumed that different regions of the grain undergo heterogeneous deformation because they interact preferentially with a different adjacent grain. In Fig. 6.5a, the upper part of the grain “feels” the presence only of the top neighbour, whereas the deformation of lower part of the grain is influenced only by the bottom neighbour. Stress equilibrium and strain compatibility can still be satisfied if a concentrated gradient appears between the upper and lower regions, creating a so-called “transition band” (Chapter 2). In such situation, replacing the top or the bottom neighbour by a grain having another orientation would only affect one half of the grain volume, conversely to what is expected in the FE simulation.

![Diagram showing grain subdividing due to preferential interaction of the upper- and lower parts of the central grain with their closest neighbour.](image)

Fig. 6.5 Grain subdividing due to preferential interaction of the upper- and lower parts of the central grain with their closest neighbour.

It is possible to estimate the orientation gradient that the transition band accommodates by applying the LAMEL model. For this, one considers separately, on the one hand, the interaction of the upper part of the grain with
the top neighbour and, on the other hand, the interaction between the lower part of the grain and the bottom neighbour (Fig. 6.5b). As the top and the bottom neighbour do not have the same orientation, the LAMEL model is susceptible to predict different $l_{13}$, $l_{23}$ and $l_{12}$ shears, respectively, for the upper and the lower part of the central grain. Consequently, the two parts are susceptible to undergo heterogeneous lattice rotations, giving rise to an intra-granular orientation gradient. In these simulations, no account is taken of a possible interaction between the two parts of the central grain (across the transition band). Therefore, the predicted orientation gradient is an upper-bound estimate of reality.

We have checked whether a correlation exists between the orientation of the central grain and the predicted orientation gradient. For this, 1500 central grains were considered, each having two neighbours with different orientations. The orientation of the central grain was one of the six characteristic orientations identified by OIM, whereas the orientations of the neighbours were selected out of a random texture. The final mean orientation of each central grain was computed by averaging the orientations predicted for its lower and upper parts. Supplementary to the intra-granular orientation spread, we have computed the average misorientation between the final mean orientation of the central grain and its initial orientation, as well as the average misorientation between any two final mean orientations of the central grain. The results shown in Fig. 6.6 correspond to 15% and 40% rolling reductions, and they indicate that:

- The orientation effects on subdivision are much stronger here than when applying FE modelling. The intra-granular orientation spread is largest for TD-rotated cube and cube and it is lowest for the β-fibre orientations where it decreases from copper to brass.

- The average misorientation with respect to the initial orientation is ~1.5 times larger than the corresponding intra-granular orientation spread. The average misorientation between any two central grains is ~1.25 larger than the intra-granular orientation spread.

- Independent of the orientation effect, all intra- and inter-granular orientation spreads are larger when predicted with the LAMEL model than when applying FE modelling.
Intra-granular orientation spread (avg miso of the upper and lower parts of the central grain relative to its mean orientation)

Avg miso between the central grain final orientation and the initial orientation

Inter-granular orientation spread (avg miso between any two of the central grain final orientations)

Fig. 6.6 Summary of the 40% rolling simulation made with the LAMEL model. (See legend.)
1.3 Discussion - Comparison to the OIM results

From this analysis, it appears that the two models that were most successful for the macroscopic texture predictions yield valid predictions also at the level of individual grains. The experimentally observed trend that grains oriented near cube develop larger orientation gradients than grains oriented along the β-fibre (Chapter 5) was found also in the simulation results. Some remarks should nevertheless be made.

According to both models, the largest orientation gradients arise in grains with a TD-rotated cube orientation because these grains show the most “unstable” orientation path, i.e. the lattice rotation within such grains is significantly influenced by the grain neighbourhood. The OIM analysis also revealed large orientation spreads within grains of TD-rotated cube orientation, but this was attributed to the formation of cell blocks with high alternating misorientations. It is possible that the tendency of TD-rotated cube grains to undergo heterogeneous deformation, which was here revealed by analysing the interaction with neighbouring grains, also promotes cell block formation. However, simulating this requires further developments of the models as will be demonstrated in the next section.

In general, the LAMEL model predicted larger orientation gradients than the FE model did. This could be foreseen already from the analysis of the local deformation tensor in Chapter 4. In the FE simulations, grains have six direct neighbours and interactions with more distant grains also occur. Relaxations relative to the macroscopic deformation are small because the individual effects of the neighbours are partly cancelled out and because large relaxations are impeded by reaction stresses in at least one not favourably oriented neighbour. Conversely, if the two neighbouring grains considered by the LAMEL model have opposite effects on the deformation of the central grain, these effects add up instead of being cancelled out. Therefore, the orientation gradient predicted between the upper and the lower parts of the central grain is generally larger than in the FE predictions. The physical interpretation of this comparison is that a larger orientation spread can be created by preferential interactions with a direct neighbour than by a continuous gradient over the grain diameter.

(1) Indeed, the average misorientation between adjacent points of the OIM grid (\( \bar{\theta}_{rel} \) or \( \bar{\theta}_{CB} \)) was larger in these grains than in grains with other orientations.
Experimentally, the line-scans shown in Fig. 5.10 revealed misorientations as high as ~20° with respect to the grain mean orientation. Such orientation gradients were found to build up over approximately one fifth of the grain diameter (i.e. over ~20µm) and they often appeared close to grain boundaries and triple junctions. According to the present simulations, misorientations of this level occur only if some grain regions interact preferentially with their direct neighbour. In the absence of such preferential interactions, the orientation gradient is expected to be smaller than 6° after 40% rolling (c.f. results of the FE simulations in Fig. 6.3). (1)

The orientation gradients predicted for grains with the brass orientation were very low. Thus, the simulations do not support the idea which was proposed in the discussion of Chapter 5 in order to explain the large gradients in some grains oriented near brass. According to this idea, grains oriented near brass are likely to undergo severe RD-TD shear but this shear may be impeded in some grain regions due to important reaction stresses from some direct neighbours. Apparently, this does not take place in the present simulations because no neighbour counteracts the RD-TD shear sufficiently. Note that the insufficiency of the constraints against RD-TD shear has already been outlined in Chapter 4 when simulating the macroscopic texture evolution.

Finally, one must note that during the FE simulations, large orientation gradients developed in grains oriented far from the six characteristic orientations considered. This trend was also revealed by the OIM analysis. It is partly due to the fact that some of these grains lie in very divergent regions of the orientation space (Dillamore and Katoh, 1974).

2 Modelling the interaction of two subgrains with the LAMEL model

The LAMEL model can easily be adapted so that it considers interactions between subgrains instead of grain interactions. There are only two differences with respect to the original version: (i) the interacting entities have originally a

(1) In fact, preferential interactions with one direct neighbour are also possible under FE modelling. However, it requires that the grains be finely discretised and that their spatial arrangement be less regular than in the simulations performed in Chapter 4.
common orientation (because they originate from the same grain), and (ii) the banded subgrains are not necessarily parallel to the rolling plane.

Leffers (1991) and Lee and Duggan (1993) were the first to suggest that banded subgrains, such as cell blocks and deformation bands, should be subjected to alternating opposite shears (see section 3.2 in Chapter 3). This idea is supported by three experimental observations: (i) within a grain, successive banded subgrains often show alternating misorientations, (ii) less than five slip systems seem to be activated in the bulk of individual grains, and (iii) cell blocks and deformation bands seem to achieve the macroscopic deformation collectively at the grain scale.

However, continuum theories do not explain how the subdivision by opposite shears is triggered (already discussed in Chapter 3): at the onset of subdivision, the energy that would be dissipated if the two subgrains underwent opposite shears is exactly equal to the energy that is dissipated under full constraints. There is thus no driving force for splitting when the two interacting entities have exactly the same orientation.

In the real material, subdivision is likely to be triggered by dislocation interaction (i.e. dislocation patterning). Indeed, (i) the width of the banded subgrains is of the order of the dislocation “mean free-path”, and (ii) cell blocks are originally formed parallel to the most stressed slip plane. Seefeldt et al (in press) are presently working on a model that is based on dislocation/disclination inter-dynamics, and that could be coupled to the LAMEL model for simulating the subdivision into cell blocks. The dislocation/disclination model will be used to predict at which strain and in which grains cell block formation is triggered. It will also provide (i) the initial misorientation between the banded subgrains, and (ii) the directionality of the bands.

Even though this crucial information is not yet available, it is interesting to test the LAMEL model under the following simplifying assumption. Let us analyse what happens if subdivision is triggered simultaneously in all grains with banded subgrains either parallel to the rolling plane (“deformation bands”) or tilted at 45° around TD (“cell blocks”). The initial misorientation is chosen to be equal to 3°, and the LAMEL model is used to predict in which grains this misorientation has most increased after 15% rolling reduction. The initial misorientation is a significant parameter in such simulations. Therefore, the
subdivision of each grain has been simulated seven times, using seven different axes for generating the initial $3^\circ$ misorientation $^{(1)}$. At the end of the simulations, the average misorientation between the seven pairs of subgrains was computed.

The results corresponding to the subdivision into deformation bands parallel to the rolling plane are presented in Fig. 6.7a. One observes that grains oriented near stable texture components ($S$ and copper) do not have the tendency to subdivide: the final misorientation between the banded subgrains is less than $3^\circ$. The opposite is true for grains oriented in “divergent” regions of the Euler space (section 3.1 in Chapter 3), with e.g. misorientations larger than $25^\circ$ for grains initially oriented near $\{111\}\langle110\rangle$. Supplementary to this, the misorientation between the subgrains tends to be larger in grains having a very high Taylor factor under plane strain compression (Fig. 6.7b). This is consistent with the experimental observations by e.g. Fortunier and Driver (1987), Duggan (1999) and Hutchinson (1999) (see section 2.2 in Chapter 2).

$^{(1)}$ The coordinates of the axes (in the sample reference system (RD,TD,ND) are: $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(1,1,1)$, $(-1,1,1)$, $(1,-1,1)$ and $(1,1,-1)$. One half of the grain was rotated $+1.5^\circ$ and the other was rotated $-1.5^\circ$.
The same type of simulations was carried out for predicting the subdivision into cell blocks oriented at 45° to the rolling plane. This second set of simulations did, however, not lead to realistic results. With almost no exception, the LAMEL model predicted one half of the grain to accommodate twice the macroscopic deformation $L_{ij}$ whereas the other half had zero strain.

This unexpected behaviour is illustrated in Fig. 6.8 and it can be explained by making the following observations:

1° It is possible that a subgrain undergoes zero strain only if its relaxation is exactly opposed to the macroscopic strain. Such relaxation is allowed here, which is demonstrated by applying a rotation of 45° around TD to the strain tensor that corresponds to the relaxation $\gamma_{13}^L$:

$$
\frac{-\sqrt{2}}{2} 0 \frac{\sqrt{2}}{2} 0 0 \frac{\gamma_{13}^L}{2} 0 \frac{-\sqrt{2}}{2} 0 \frac{\sqrt{2}}{2} 0 \frac{\gamma_{13}^L}{2} = \frac{-\gamma_{13}^L}{2} 0 0 0 \frac{-\gamma_{13}^L}{2} 0 \frac{\gamma_{13}^L}{2} 0 0 \frac{\gamma_{13}^L}{2}
$$

The rotated relaxation tensor compensates exactly the macroscopic strain when $\gamma_{13}^L$ is equal to $2L_{11}$.

2° As the second subgrain undergoes opposite shear, its relaxation adds up to the macroscopic strain, yielding $l_{ij}=2L_{ij}$. This ensures that the average deformation of the two subgrains is equal to the macroscopic deformation: $(2L_{ij}+0)/2 = L_{ij}$.

3° Under plane strain compression, the deforming subgrain has a lower Taylor factor than the non-deforming one (this difference results from the initial misorientation of 3°). If we denote the deforming and non-deforming grains with the indices $I$ and $II$ respectively, the dissipated energy is $2M^d + 0$ which is smaller than the energy dissipated under full constraints: $M^d + M^d$ (because $M^d<M^d$). This reduction of the dissipated energy is the driving force of subdivision.

4° Finally, one should note that the grain region undergoing zero strain has a non-zero anti-symmetric part of the velocity gradient tensor, thus a non-zero lattice rotation.
Fig. 6.8 Plane strain compression of two cell blocks tilted at 45° to the rolling plane (longitudinal view). a) Original shape of the subgrains. b) Prediction of Taylor FC (i.e. macroscopic deformation). c) Illustration of a $\gamma_{13}^L$ relaxation that is exactly opposed to the macroscopic deformation (in the upper subgrain).

Experimentally, the two cell-block families seem however to have similar strains: the dislocation density and the average cell-size are similar in both families. In fact, the present LAMEL simulation better corresponds to the deformation mechanism observed experimentally in shear bands and in copper microbands. In those cases, the localised shear is even larger than in the present simulation because the shearing volume is much smaller than the non-deforming volume.

It is likely that better predictions of cell-block subdivision require the introduction of some hardening. This will be attempted when coupling the LAMEL model to the Seefeldt et al (in press) model.
In this thesis, several polycrystal plasticity models have been used to simulate the development of rolling textures and the occurrence of intra-granular heterogeneities of strain, stress and lattice orientation. The purpose was to investigate whether classical polycrystal plasticity theories could advantageously be replaced by “N-site” models in which the interaction between adjacent grains is accounted for.

Four models have been selected for the comparison. The “full constraints” (FC) Taylor model and the “relaxed constraints” (RC) pancake model are classical theories of plasticity. Both models oversimplify reality by assuming that the deformation is homogeneous within each grain, and that any two grains with the same initial orientation should deform in the exact same way. These limitations are overcome by the two other models, according to which grains have a specific neighbourhood that influences the grain deformation and creates in-grain heterogeneities. In the LAMEL model, interactions are assumed to involve only two grains at a time, and local deviations relative to the macroscopic deformation are restricted to pure shears parallel to the rolling plane. In the more elaborated finite element (FE) model, all components of the local deformation tensor may vary so as to fulfil stress equilibrium and strain compatibility over the whole polycrystalline aggregate.

The four models have first been applied to the prediction of the macroscopic rolling texture. It was necessary to develop new tools for texture characterisation and texture modelling:

- A new procedure has been developed for a quantitative characterisation of the crystallographic fibres appearing in fcc and bcc rolling textures. The fibres are located more accurately than previously, and their strength is measured by computing integrals of the ODF-intensity in sections perpendicular to the fibre. Such integrals better correlate to the physically meaningful volume fractions than the traditionally used ODF-value at the
fibre centre. Furthermore, the integrals are more relevant when comparing textures in which the fibre is slightly shifted.

- The software implementation of the LAMEL model initially available for this work was plagued by incessant convergence problems. Hence, the method used for solving Taylor ambiguity had to be replaced. The new procedure determines all combinations of slip rates which satisfy the geometrical constraints while dissipating minimum energy. The slip rate combination that is used subsequently for computing the lattice rotation is the linear combination of all valid solutions, which fulfils a criterion defined by the operator.

- In order to improve texture predictions in aluminium, the LAMEL model had to be adapted. The new version of the LAMEL model includes a supplementary type of relaxation: RD-TD shears. The no-grain-boundary-sliding condition is satisfied by requiring that the two grains, which are separated by an interface parallel to the rolling plane, undergo the same RD-TD shear.

Six plates (two made of steel and four of aluminium) rolled to moderate and high strains have served as reference for the simulations. The following conclusions could be drawn:

- The new method for texture characterisation was first applied to the ODFs derived from experimental measurements on the various steel and aluminium plates. According to this analysis, the initial texture has a significant influence on the texture developing in the material upon rolling.

- The LAMEL model provided the best predictions of the steel rolling textures closely followed by the FE model. The strength of the γ-fibre was reproduced quantitatively, which is absolutely not true when classical plasticity theories are applied.

- The FE model was most successful in reproducing the aluminium textures. The revised version of the LAMEL model also led to improved predictions compared to the classical plasticity theories. The predictions of the FC Taylor model were found to depend significantly on the criterion applied for solving the Taylor ambiguity.

- An analysis of the local deformation tensor predicted by the various models has shown that the shear relaxations predicted by the LAMEL
model were halfway between the shears predicted by the RC pancake model and those predicted in the FE simulations. Furthermore, it is the same deformation tensor components that fluctuate most over the FE mesh and that are relaxed in the LAMEL and the RC simulations.

- In the LAMEL simulations, grains interact with only one direct neighbour. The dislocation activities of the interacting grains are strongly correlated with one another and a microtexture builds up. In some cases, the two grains rotate towards end-orientations that are symmetric relative to the rolling plane. In other cases (other end-orientations), the opposite trend is found: grains seem to avoid being associated with their mirror orientation.

On the whole, the results of the texture predictions are very encouraging. The models accounting for grain interactions always performed better than the classical theories of plasticity. Although it requires much less computing time than the FE simulations, the LAMEL model reproduces the experimental texture development almost as closely as the FE model does.

The second important question that has been addressed in this thesis is to determine whether the assumptions made by the LAMEL and/or the FE model about direct neighbour interactions can be validated from microstructural observations at the grain-scale. As no existing experimental technique permits recording the deformation history of grains imbedded in the bulk of a polycrystal, traces of grain interaction effects must be sought in the intra-granular orientation gradients and dislocation patterns. Therefore, a statistical analysis of grain subdivision in cold rolled aluminium (AA1050) has been carried out. This study relies on orientation imaging microscopy (OIM) in the SEM, and it is complementary to the abundant earlier TEM investigations because larger sample surfaces are here covered. The analysis led to the following results:

- Although the resolution of the SEM/OIM technique is low compared to TEM, OIM may be successfully used for observing grain subdivision and the development of in-grain orientation gradients in moderately deformed materials. The characteristic cell block subdivision pattern that is reported in numerous TEM studies has been resolved by OIM in certain grains of the 40% cold rolled aluminium. The results seem to indicate that for identifying micrometer sized cell blocks, the angular accuracy of EBSD measurements is more critical than the spatial resolution.
A new procedure has been proposed for a quantitative analysis of grain subdivision from OIM data. The procedure is based on the computation of two average misorientations characterising the overall orientation spread within each grain as well as the occurrence of subgrain boundaries accommodating a large orientation change.

The computational procedure has been applied to 16 orientation maps covering more than 400 grains. The results demonstrate that grains with different orientations show different in-grain heterogeneities. (i) Grains oriented close to the cube \{001\}<100> and RD-rotated cube \{025\}<100> components develop orientation gradients over distances of 10 – 20 µm. (ii) Grains with orientations near TD-rotated cube \{205\}<502> form fragments with relatively large misorientations, and (iii) grains with orientations along the β-fibre (S, Cube and Brass orientations) form fragments with relatively small misorientations. These orientation effects on subdivision are mostly in concordance with earlier TEM observations of aluminium single crystals and of individual grains in polycrystalline samples.

The analysis of the orientation maps has revealed significant intra-granular orientation gradients in certain grains. The formation of such gradients is likely to have a non-negligible effect on the macroscopic texture evolution.

By revealing a correlation between the mean orientation of a grain and the type/level of subdivision, the OIM analysis provides relevant microstructural information for testing plasticity models at the grain-scale. In the last chapter of this thesis, we have checked whether the “long-range” orientation gradients revealed by OIM could originate from grain interactions. A series of computational experiments have been designed in order to simulate the build up of such heterogeneities:

Applying the FE model that was already used for the global texture predictions, constant orientation gradients arise from one edge of the grain to another. For a comparison with the OIM observations, we have investigated how a given grain behaves on average in a variety of neighbourhoods. Applying the LAMEL model, it is possible to simulate the formation of so-called “deformation bands”. In this case, the orientation gradients occur because different regions of the grain interact preferentially with different adjacent grains.
Although they rely on different hypotheses, the FE model and the LAMEL model predict a relatively similar correlation between the mean orientation of the grains and the level of in-grain orientation spread. The orientation gradients are however greater when predicted with the LAMEL model. According to both models, the orientation spread is larger in grains oriented near cube than in grains oriented along the β-fibre. This trend is consistent with the experimental observations by OIM.

The validation of the models at the microstructural level is satisfactory. It is quite promising if we acknowledge the room that is left for future improvements. The applied models were originally elaborated for macroscopic simulations but we believe that these models also have the potential to simulate the local micromechanics.

**Future developments**

The present thesis leaves a number of doors open for future research. On the one hand, it would be interesting to check whether the LAMEL model performs better than classical plasticity theories for the prediction of texture dependent macroscopic properties:

- The LAMEL model could for example be applied to the prediction of the formability and the planar anisotropy of a sheet, i.e. the forming limit diagram (FLD) (Van Houtte and Toth, 1993) and the r-value profile (Schouwenaers et al, 1994). Nowadays, these properties are estimated by relying on the FC Taylor assumption, thus neglecting grain interactions.\(^{(1)}\)

- The LAMEL model could also be implemented as the material law in full-scale FE simulations of deformation processes. In such simulations, each node has the flow properties of a polycrystal that is traditionally assumed to obey FC Taylor. Implementing the LAMEL hypothesis in a macroscopic FE model would allow the simulation of deformation processes that involve complex strain paths. Some examples are: deep-drawing, hydro-forming,

\(^{(1)}\) It must be noted that 1-site models, such as the FC Taylor model, permit an extremely fast computation of the macroscopic yield locus based on an averaging rule that is proper to the series harmonics (Chapter 1). N-site models, such as the LAMEL model, do not allow this and should therefore be computationally more demanding.
rolling with redundant shear and friction at the rolls (creating through thickness texture gradients), etc.

Contrarily to the grain-scale FE model in which grains interact with many neighbours, applying the current LAMEL model is only justified when grains are pancaked (like in a rolling microstructure). More suitable models might be designed for the study of equiaxed grain, e.g. during equal channel angular extrusion (ECAE), or of grains elongated in one direction, e.g. during wire drawing. These models might consider the co-operative deformation of more than two grains at a time and they might imply other relaxation types than pure shears (1). In view of these potential developments, it should be noted that in the current version of the LAMEL model, the interacting grains undergo the same equivalent strain. This is because the macroscopic deformation and the relaxation are “orthogonal” deformation modes (Van Houtte, 1995b) which have distinct contributions to the local equivalent strain. This would not anymore be the case if the lamellas were not parallel to the rolling plane (2) or if the relaxations would involve normal strains. In the real material, it is likely that some grains are submitted to a (slightly) larger equivalent strain than others. However, such non-uniform distribution of strain can be correctly simulated with N-site interaction models only if some hardening is taken into account.

The suggested elaboration of new N-site models could efficiently be assisted by orientation imaging microscopy (OIM). The computational analysis of the local orientation data has revealed definite orientation effects on subdivision but it has also demonstrated a potential influence of the grain shape/size and surrounding (though the scatter in the $\bar{\theta}_m$ and $\bar{\theta}_{rel}$ values). This experimental investigation could be pushed one step forward by introducing supplementary parameters. One might, for example, investigate whether the orientation gradient within grains of cube orientations is different when the neighbouring grains have either higher or lower Taylor factors, or whether the orientation gradient depends on the number of direct neighbours. Such

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(1) However, only pure shear relaxations allow fulfilling the no-grain-boundary-sliding condition along the interface separating the grains.

(2) In section 2 of Chapter 6, an attempt was made to simulate cell block subdivision with lamellas inclined at 45° to the rolling plane. The consequence was that one grain underwent double equivalent strain while the other underwent zero equivalent strain.
multivariate analysis would, of course, require supplementary scans so as to increase significantly the size of the grain sampling. Evidently, it would also be interesting to perform similar analysis on other materials and/or at larger strains.

Finally, it is clear that both the LAMEL model and the grain-scale FE model still use oversimplified representations of the micromechanics. We have stressed that some grain subdivision mechanisms can be reproduced only if one accounts for dislocation patterning. In the future, an elaborated version of the LAMEL model could be constructed with a two-level architecture. It would consider (i) the interaction with neighbouring grains and (ii) the development of intra-granular strain heterogeneity. The latter heterogeneity would be triggered by dislocation interactions based on e.g. the Seefeldt et al (in press) model. It is noteworthy that coupling a grain-scale FE model to a dislocation patterning model is a much more complex task because it implies a re-definition of the FE mesh parallel to the dislocation sheets predicted from dislocation interaction.
General conclusion
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Curriculum Vitae

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