Multiscale Approaches

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Abstract. This paper presents a review of the main families of multiscale models. A first group of models is interested in an accurate modelling of the texture induced anisotropy of the material during numerical simulations. The differences between the proposed models are mainly due to different choices concerning the necessary compromise between the importance of the microscopic roots of the model and the maximum admissible computation time. The length scale of the investigated process is also an important parameter. The second group of micro-macro models is based on an analysis of the dislocation densities linked to the plastic deformations. A discussion concerning the past evolution, the recent achievements and the future trends concerning multiscale models is also provided.

Keywords: Micro-macro, texture, homogenization techniques, dislocation densities, finite element modelling.

1 Introduction

The microscopic mechanisms involved during plastic deformation of metals are various and very complex, depending on the material, the forming process and the experimental conditions investigated. Nowadays, numerous complex constitutive laws are developed in order to improve the accuracy of the finite element (FE) technique.

Sophisticated macroscopicphenomenological models (dedicated to yield locus anisotropy or/and hardening behaviour) with an increasing number of parameters are proposed. This chapter mainly focuses on another approach: the multiscale material models which are based on the physics and include more and more refined microscopic mechanisms.

Macroscopic phenomenological models are efficient for the numerical simulations of industrial forming processes (e.g. automotive industry, can forming) due to the low computation time required. However, multiscale models are very helpful for the identification of the material properties. For instance, while experimental tests provide some points on the yield locus, micro-macro models are able to compute the shape of the yield locus useful for the setting of the phenomenological models.

Accurate models based on the physics are also required for a deep understanding of the material behaviour, which is a crucial point for the development of new materials with optimum texture and microstructure and their associated forming processes. For

instance, the springback modelling after any metal sheet forming process and the earing prediction during deep drawing are still under progress.

Even if the multiscale models generally require large computation time, the continuous improvement of the computer performances permits to account for more and more refined microscopic plastic deformation mechanisms.

Section 2 presents an overview of the multiscale models where the anisotropy of the material is deduced from the crystallographic texture. The efficiency of these models generally results from a compromise between computation time considerations and the refinement of the microscopic models.

Section 3 is devoted to models taking into consideration the dislocation densities inside the crystals constituting the material. Microscopic models dedicated to small length scale modelling as well as macroscopic models with microscopic roots are presented.

Discussions, future trends and conclusions end this current review.

2 Multiscale models based on texture

2.1 General features

An important point when dealing with multiscale models is the micro-macro transition (or homogenization technique), which is necessary to deduce the macroscopic material behaviour from microscopic considerations. This step must be achieved with care because it determines the accuracy of the multiscale model.

At this stage, different scales for the analysis of the problem are defined:

- The scale of the sample: only the macroscopic stress field and strain rate field are important at that scale. They are computed by the finite element code on the basis of the lower scale analyses.
- The scale where the macroscopic fields are assumed to be constant in order to be able to achieve the micro-macro transition which is the topic of section 2.2. From a finite element point of view, this scale is the scale of one integration point of one finite element. From a physical point of view, this scale should be the smallest representative volume of the polycrystal behaviour. A sufficient number of crystals must be included in this volume to correctly represent the material texture.
- The scale of the crystal or the microscopic scale: a microscopic material model (based e.g. on dislocation sliding) must be developed at this scale. It is the starting point for the micro-macro transition.
- The dislocation pattern scale: this scale is larger than a single dislocation but smaller than the crystal scale. The interaction between dislocations, the presence of obstacles or substructures inside one grain are analysed at this scale. The microscopic events linked to this length scale are more deeply analyzed in section 3.
- The atomistic scale: this scale is not considered here even if dislocations dynamic simulations have given lots of new insights into the elementary processes of the dislocation motions and their interactions that define the dislocation patterning [1-3].

The smallest scale considered in this section is the scale of the crystal called the microscopic scale. The micro-macro transition results from the averaging of the microscopic values over the representative volume element (RVE):

$$\underline{\underline{\sigma}}^{macro} = \frac{1}{V} \int_{RVE} \underline{\underline{\sigma}}^{micro} dV \ , \tag{1}$$

$$\underline{\underline{\dot{\varepsilon}}}^{p,macro} = \frac{1}{V} \int_{RVE} \underline{\underline{\dot{\varepsilon}}}^{p,micro} dV \ . \tag{2}$$

With the use of $f(g)$, the orientation distribution function (ODF), one has:

$$\underline{\underline{\sigma}}^{macro} = \int \underline{\underline{\sigma}}^{micro}(g) \ f(g) dg \ , \tag{3}$$

$$\underline{\underline{\dot{\varepsilon}}}^{p,macro} = \int \underline{\underline{\dot{\varepsilon}}}^{p,micro}(g) \ f(g) dg \ , \tag{4}$$

the integration being done over all the possible orientations of the crystals.

Even if the relation between microscopic stress and plastic strain rate is known, the corresponding relation at the macroscopic level is not straightforward. The averaging over all the crystallographic orientations seems a very simple concept but it must be done simultaneously on the stress and the plastic strain rate because of their interaction in the single crystal. A solution to this problem is then very hard to find and is discussed in section 2.2.

2.2 Homogenization techniques

Several methods have successively been proposed in order to solve the micro-macro transition. The main ones are:

Sachs' model. Based on [4], one has derived the assumption of a homogeneous stress distribution throughout the whole polycrystal. The stress in each crystal is then chosen equal to the macroscopic stress. The averaging must then only be achieved on the plastic strain rate. This model is not very satisfactory and gives rise, in the general case, to a contradiction. Indeed, each crystal having its own orientation, imposing a common stress expressed in the sample coordinate system to all the crystals consists in imposing a different stress to each crystal in its reference system. The yield locus of each crystal being quite anisotropic, the imposed stress cannot fall on the yield locus for each crystal. One can understand that no compatibility of the strain rate will be fulfilled between neighbouring grains with such an approach. This model is generally not implemented in FE method.

The full constraints (FC) Taylor's model [5]. According to literature, Taylor type models are the most widely used for the computation of the constitutive response of

polycrystal aggregates. Taylor's model assumes a homogeneous distribution of the velocity gradient trough the polycrystal. This assumption is expressed for each crystal by:

$$\underline{\underline{L}}^{micro} = \underline{\underline{L}}^{macro} \quad . \tag{5}$$

Within a finite element code when elasticity is neglected, the plastic strain rate is the symmetric part of the velocity gradient $\underline{\underline{L}}$:

$$\underline{\underline{\dot{\varepsilon}}}^{p,macro} = \frac{1}{2}\left(\underline{\underline{L}} + \underline{\underline{L}}^{T}\right) \quad \text{, with} \quad \underline{\underline{L}} = \frac{\partial \underline{v}}{\partial \underline{x}} \ , \tag{6}$$

where $\underline{v}$ is the velocity field and $\underline{x}$ is the spatial coordinates.

Thanks to Taylor's assumption, the micro-macro transition can easily be implemented into a finite element code. The velocity gradient is given by the finite element code at each integration point and the corresponding stress is sought for. The plastic strain rate is deduced from equation (6) in a macroscopic point of view; the microscopic one is identical for all the crystals of the RVE associated with one integration point (see equation (5)), however it must be rotated to be expressed in each crystal lattice reference system. Each crystal in its own reference system sustains a different plastic strain rate. The microscopic stress is computed for each crystal from its yield locus. The macroscopic stress of the polycrystal is obtained by a weighted averaging of the microscopic ones with the use of the ODF as shown by equation (3).

This procedure consumes computation time if a large number of crystals is considered. Anyway, it offers the advantage that each crystal is treated successively and independently of the other crystals. So, multiprocessor computation can easily be applied. As the Voigt's model is an upper bound for the elastic stiffness matrix, the Taylor's model is an upper bound for the yield stress. The stress equilibrium between individual grains is generally violated with the Taylor's model.

According to literature (see e.g. [6]), in spite of its limitations, this model appears to be quite successful in the prediction of the stress-strain response of the polycrystal and of the texture during plastic deformations. It is however widely recognized that the textures predicted by Taylor type models are much stronger than the actual measurements.

The relaxed constraints (RC) models [7-9]. Taylor's assumption of a homogeneous plastic strain rate in the RVE is, in some applications, too restrictive. From a physical point of view, nothing ensures that the plastic strain rate is constant in a crystal and identical in all the neighbouring crystals; it is not even sure that the plastic strain rate is close from one crystal to another. According to the considered forming process, it is interesting to modify the assumption of a homogeneous plastic strain rate. In the case of rolling, the X-axis being the rolling direction, the Y-axis being the transverse direction and the Z-axis being the normal direction, the lath model relaxes the XZ component of the plastic strain rate. The relaxed component is no more identical for all the crystals but is free. The pancake model relaxes in addition the YZ component. The lath and pancake methods seem to be more satisfactory for the modelling of the roll-

ing process than the FC Taylor's model (particularly for the prediction of the deformation textures), they take into account the elongated shape of the crystals.

Note that the compatibility conditions disappearing on the relaxed plastic strain rate components must be replaced by equilibrium conditions on the corresponding stress components.

The main disadvantage of these relaxed models is that they are dedicated to a particular forming process; they cannot be used for an arbitrary strain history. The generalised relaxed constraints method (see [10]) overcomes this drawback by choosing automatically the plastic strains that should be relaxed.

The multiple points models: as it has been explained, due to their assumptions, the previous models treat each crystal in turn. Interesting from a computational point of view, this choice increases the difficulty to take into account the effect of the interaction between adjacent crystals. That is the reason why multiple points models have been investigated. For instance, the Lamel model [11-13] examines the interaction between 2 grains still assuming rolling simulation. The flattening and the elongation of the rolled crystals led to the idea of considering 2 grains having the same size and shape and which lie exactly on top of each other. The boundary between these 2 grains being parallel to the plane of the steel sheet. The FC Taylor's condition of uniform plastic strain rate is here applied to the set of the 2 grains and not to each grain. Under such conditions, the crystals have 2 relaxations: the XZ and the YZ components of the velocity gradient are relaxed (using the same coordinates as above). Now, the relaxation of the top grain must be the opposite of the relaxation of the bottom grain, which is different from the RC models. The stress equilibrium between the 2 grains must be verified. Table 1 of [13] shows that the Lamel model predicts more accurately the deformation texture than the RC or the FC Taylor's models. A stack of 3 grains instead of 2 is also proposed by [13]. A more recent Lamel version with, in addition, the relaxation of the XY component has also been investigated [12].

Figure 1 schematically compares the FC Taylor's, the Lamel and the pancake models. Opposite shear appears with the Lamel model (computed by minimization of the total plastic work rate in the two grains). No shear appears with the FC Taylor's model because it is prescribed in a macroscopic point of view while the pancake model violates the compatibility between both grains.

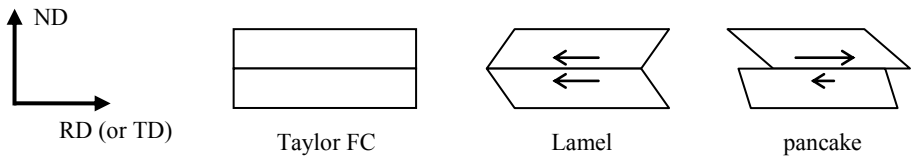

Figure 1: Comparison of the FC Taylor's, the Lamel and the Pancake models (adapted from Fig. 1 of [13])

The GIA (Grain Interaction model) [14] is similar but more general than Lamel model. It considers the interaction between 8 grains. The relaxed shear components are as in the Lamel model. This model is not limited to the rolling deformation mode; but it requires larger computation time.

In the Lamel model, the interfaces between two adjacent grains must always be parallel to the RD – TD plane. This constraint limits this model to rolling processes. In the recent Advanced Lamel (ALAMEL) model [15], the orientations of the interfaces are defined either by the user as a function of the material and the process investigated or they can be randomly chosen with a rule taking into account the grain shape. Therefore, the ALAMEL model is suitable for any deformation mode.

The self-consistent model (see [16-17]). It is a generalisation of the multiple points models in the sense that all the crystals are treated as if they would act simultaneously. The self-consistent model considers each grain in turn as an inclusion embedded in an ideal homogeneous plastic matrix. As this plastic matrix is expected to represent the polycrystal behaviour, it is obtained by an averaging of the single crystal behaviour. An iterative procedure must be used. From a computational point of view, Taylor's model, for instance, is used to obtain a first approximation for the matrix behaviour. Each grain is then computed as the inclusion into that matrix. The new matrix behaviour is obtained by averaging on all the grains. The computation is repeated until convergence is obtained on the matrix behaviour. With this model, the stress and the plastic strain rate are allowed to be different from one grain to another (the assumption of uniform stress and plastic strain rate inside each crystal is however kept). This model should conceptually be more accurate than the previous ones but requires larger computation time. However, on a local point of view, neither equilibrium nor displacement compatibility are fulfilled.

Note that a first trial of a self-consistent approach was Kröner's model [18]. On the basis of Eshelby's work, Kröner treats the problem of a spherical plastic inclusion representing one crystal embedded in an elastic matrix. The polycrystal behaviour is the average on all the crystals. The plastic incompatibility between the crystals is accommodated elastically. As a consequence, this model overestimates the yield stress just like Taylor's model. Moreover, as the matrix is assumed to be purely elastic, it cannot correctly represent the polycrystal behaviour. In that sense, Kröner's model is not literally a self-consistent model.

A visco-plastic self-consistent polycrystalline model [19] implemented in a 3D FE code extends previous versions limited to elasto-plasticity towards actual elasto-visco-plastic behaviour (see also [20]).

An original micro-macro model based on a solid volume fraction internal variable approach and a self-consistent approximation is presented in [21] to describe the isothermal steady state flow behaviour of semi-solid material (thixoforming) in a large range of strain rates. A specific self-consistent model based on the integral equation for the translated visco-plastic strain rate field is proposed in [22].

Pilvin's model [23]: in order to be able to simulate complex path loading, starting from Kröner's model, Pilvin added accommodation variables (β-law). A 2 stage complex mathematical formulation is used for the micro-macro transition. The physical meaning of this model is not clear; nevertheless, it compares favourably to other models.

2.3 Micro-macro models without macroscopic yield locus

A large class of models assumes that a set of representative crystals is associated to each integration point of a macroscopic FE mesh. For each crystal, an elasto-plastic or elasto-visco-plastic crystal plasticity model is chosen and the homogenization technique takes care of both the average process to provide the macroscopic answer and the identification of the microscopic quantities [24-25].

The crystal plasticity finite element method (CPFEM) [6;26-27]: In this method, each finite element represents one grain of the polycrystal. The constitutive law for one particular element is then the microscopic law governing the crystal behaviour. In order to model the polycrystal behaviour, each finite element corresponds to a particular crystal orientation so that the ODF of the material is correctly represented by the whole finite element mesh. A particular procedure must be used to assign one specific orientation to each finite element of the mesh.

Note that some variants of this model are proposed: one finite element can represent more than one grain (for instance, each integration point is assigned a different lattice orientation; if each element contains 8 integration points, it has 8 different lattice orientations, i.e. each element is assumed to be made of 8 grains). On the other hand, each element of the finite element mesh can represent a region smaller than a grain; one grain is then modelled by several finite elements. Other variants have also been investigated (by e.g. [6]).

The main advantage of this model is that it simultaneously ensures stress equilibrium and deformation compatibility between grains. It is basically the goal of the finite element technique. This point has been proved to be a significant improvement compared to the Taylor's model. Large deformation heterogeneities between grains have indeed been observed with the finite element technique (as shown by Figure 2).

Figure 2: Deformed finite element mesh from the simulation of plane strain compression on model 3D-400E-400g2 to a 70% reduction level (ε=-1.2). From [6].

Unfortunately, this method requires larger computation time than the Taylor's model. For the finite element simulation of a complex forming process, this technique can hardly be used. Indeed, for this method, one finite element has a length scale of the order of the size of one crystal. While the global mesh has the size of the sample. A very large number of elements should be used in most cases of actual forming processes.

Nevertheless, a multi-level FEM approach or FEM^2 method [28-31] would allow to avoid (or reduce) the problem of the previous approach. Two distinct finite element meshes are used. The first one is a macroscopic mesh (at the scale of the sample) representing the forming process. The second finite element mesh is a microscopic one and is used to achieve the micro-macro transition. The size of that mesh is of the order of the representative volume element, i.e. the number of elements of this second mesh

must be such that the ODF is correctly represented. Such a microscopic finite element mesh is then supposed to be placed at each integration point of the macroscopic mesh. One complete computation at the micro level must then be achieved each time an integration point of the macro level is treated. Anyway, due to the large length scale difference between the two meshes, the overall number of elements and nodes in the FEM^2 method (on both scales) is expected to be lower than for the CPFEM.

The multisite model [32-34] of Delannay adopts a different strategy. It assumes (i) that the deformation of each grain is predominantly influenced by short-range interaction with adjacent grains, (ii) that local strains deviate from their macroscopic average according to specific relaxation modes, and (iii) that the macroscopic strain is achieved on average by every pair of adjacent grains.

The model bears some resemblance with the Lamel model. However, as it is a severe limitation of the Lamel model, the relaxation modes in the multisite model do not assume that grain boundaries are aligned with the rolling plane. Instead, as in the Alamel procedure, the grains interact across a planar interface that is not necessarily parallel to the rolling plane. The relaxation modes in the multisite model are defined by the user, so that the model can either reduce to the full constraints Taylor's model, the pancake, Lamel or Alamel models. According to the finite element mesh and the way to represent the texture of the material, multisite model is able to achieve a CPFEM analysis.

The large flexibility of the multisite model allows generating different micro-macro models; on the other hand, large computation time is generally required during FE simulations.

The method proposed by Dawson and Kumar [35-38] is based on two coupled FEM analyses. A classical mechanical analysis is applied at the scale of the forming process. The texture computation relies on a second FEM analysis in the crystal orientation space. The ODF is described by a FE mesh in order to compute the texture evolution by solving the ODF conservation equation [39].

2.4 Micro-macro models with macroscopic yield locus

The computation time for the models presented in previous section is generally very large when industrial forming processes are investigated. Therefore, micro-macro models with a macroscopic yield locus were developed. The macroscopic yield locus is employed during the FE computation in order to reduce computation time. This yield locus is determined from the micro-macro model either in a pre-processor or during the FE computation.

To define the macroscopic yield locus, Van Houtte and Van Bael [40-41] proposed to use the rate of plastic work per unit volume as plastic potential in the strain rate space. The yield stress (expressed as a vector in 5D space) is the first derivative of the potential:

$$\underline{S} = \frac{\partial \Psi}{\partial \underline{D}} \ . \tag{7}$$

A 6th order series expansion is used to approximate the plastic potential:

$$\Psi\left(\underline{D}\right) = \tau D\sqrt{\frac{2}{3}}\bar{M} \approx \tau D F_{pqrstu}\frac{D_p}{D}\frac{D_q}{D}\frac{D_r}{D}\frac{D_s}{D}\frac{D_t}{D}\frac{D_u}{D} \quad , \qquad (8)$$
$$with\, 1 \le p \le q \le r \le s \le t \le u \le 5$$

where D is the norm of the strain rate $\underline{D}$ defined in 5D space; τ characterizes the hardening and $\bar{M}$ is the average Taylor factor. The computation of the 210 series expansion coefficients F_{pqrstu} is achieved by a least square fitting based on average Taylor factor or, more efficiently, using a linear method based on texture C-coefficients with pre-calculated libraries.

As the convexity of the 6th order formulation of (8) is not guaranteed, according to the modelled material, so called fish-tails, particularly inconvenient during FE simulations, are sometimes encountered. Therefore, a new version of the 6th order potential was proposed [42]:

$$\Psi\left(\underline{D}\right) = \tau D\sqrt{\frac{2}{3}}\bar{M} \approx \tau\sqrt[6]{\alpha'_{pqrstu}D_pD_qD_rD_sD_tD_u} \quad . \qquad (9)$$
$$with\, 1 \le p \le q \le r \le s \le t \le u \le 5$$

The calculation of the 210 series expansion coefficients α'_{pqrstu} is achieved by a three step iterative procedure that ensures strict convexity.

Similarly, Arminjon and co-workers [43] used a 4th order series expansion to define a macroscopic yield locus. This formulation was implemented in a finite element code [44-45] to simulate deep drawing of steel and aluminium.

Darrieulat and Montheillet [46] proposed a methodology to derive a quadratic yield function for orthotropic aggregates of cubic crystal from the associated texture components. The parameters of Hill's quadratic yield locus are determined by averaging the functions corresponding to the individual texture components of the investigated material's texture.

Maudlin and co-workers [47] have investigated such an approach with a yield locus approximated by a set of hyperplanes (plane in 5 dimensional deviatoric stress space). They called the fitting procedure "tessellation", highlighting the fact that the continuity between the hyperplanes must be fulfilled, i.e. the yield locus must be a continuous surface. The tessellation is achieved on 647 stress points that are calculated on the basis of the texture of the material using a visco-plastic self-consistent model [19] assuming a combination of prismatic and pyramidal slip systems [48]. 1226 linear functions defining the hyperplanes are then obtained. The yield locus is described with a continuous mathematical formulation with sufficient detail to be integrated in a finite element code.

The Minty model developed by Duchêne and Habraken [49] is a crystal plasticity law adapted to macroscopic forming processes simulations. This law is based on a local yield locus approach able to predict texture evolution during FE modelling of industrial forming processes. With this model, only a small zone of the yield locus is

computed. This zone is updated when its position is no longer located in the part of interest in the yield locus or when the yield locus changes due to texture evolution.

This model is specific in the sense that it does not use a yield locus formulation either for plastic criterion or in the stress integration scheme. A linear stress-strain interpolation in the 5-dimensional (5D) stress space is used at the macroscopic scale:

$$\underline{\sigma} = \tau \underline{\underline{C}}.\underline{u} \ . \tag{10}$$

In this equation, $\underline{\sigma}$ is a 5D vector containing the deviatoric part of the stress; the hydrostatic part being computed according to an isotropic elasticity law. The 5D vector $\underline{u}$ is the deviatoric plastic strain rate direction (it is a unit vector). τ is a scalar describing an isotropic work hardening.

The macroscopic anisotropic interpolation is included in matrix $\underline{\underline{C}}$. Its identification relies on 5 directions: $\underline{u}_i$ (i=1…5) advisedly chosen in the deviatoric strain rate space and their associated deviatoric stresses: $\underline{\sigma}_i$ (i=1…5) computed by the polycrystal plasticity model. This micro-macro model uses Taylor's assumption of equal macroscopic strain and microscopic crystal strain. It computes the average of the response of a set of representative crystals evaluated with a microscopic model taking into account the plasticity at the level of the slip systems. Two versions of this Full Constraints (FC) Taylor's model are investigated: one coupled with a rate insensitive crystal plastic model and one coupled with a visco-plastic crystal model in [50].

Texture evolution is computed using Taylor's model on the basis of the strain history for each integration point every 10 FE time steps. This law is very modular and the principle of this approach can be coupled with any microscopic model and homogenization technique. Further details and properties of Minty law can be found in [49].

Minty and the 6th order yield locus (fitted on Taylor and Lamel models) are compared during deep drawing simulations in [51].

3 Multiscale models based on dislocation densities

3.1 Description and main features

Multiscale models based on dislocation densities can have a strong macroscopic character: the FE mesh has macroscopic scale and the constitutive law relies on balance equation of different mechanisms of generation and annihilation of dislocations, see for instance the models of Pietrzyk [52-53] or Kopp [54]. Microstructure evolution can also be followed by such an approach, when the link between dislocation densities and phase transformation [55-56] or recrystallization [57] is clearly identified.

Another type of dislocation models looks at a smaller scale. The assumption of uniform stress and strain distribution inside each crystal can yield to inaccurate results depending on the material and the process investigated. In particular, when the dimensions of the sample are of the same order than the length scale of the microstructure (the grains size), the new generation of strain-gradient crystal plasticity models are of great interest [58].

Hereafter only a few examples are provided.

3.2 Microscopic models

The internal variable model of Pietrzyk [52-53] is based on the computation of the stress during plastic deformation as a function of the evolution of dislocation populations controlled by competition between storage and annihilation of dislocations. Various models for the description of the dislocation density evolution were proposed. In this respect, a simplified analytical solution of differential equation is proposed in [59]. Models with only one internal variable: the average dislocation density [60] or with two internal variables: the densities of mobile and trapped dislocations [61] were investigated. Finally, a complex model based on the distribution of dislocation density function was developed [53]. This full model accounting for the distribution of dislocation density provides accurate predictions during hot forming of metals [57] but requires larger computation time during FE simulations.

Geers and co-workers proposed a crystal plasticity model [62] on the polycrystal scale which considers each grain as a single crystal core surrounded by flat bi-crystals representing the grain boundaries. When the polycrystal plastically deforms, due to the bi-crystal interface conditions (stress equilibrium and deformation compatibility), the bi-crystals and the crystal core will behave differently. This heterogeneous behaviour gives rise to the generation of geometrically necessary dislocations (GND) in order to fulfill crystallographic lattice compatibility. These GND's act as obstacles to the motion of the statistically stored dislocations (SSD), which carry the plastic deformation.

In order to improve the model, the heterogeneities within each grain were afterwards considered at the single crystal level [63-64]. Therefore, each grain had to be modelled with a sufficient number of finite elements (around 20 in [64]). GND's and SSD's are still accounted for, while grain boundary dislocations (GBD) densities are added in order to consider the initial lattice mismatch between adjacent grains. Application of this model to constrained simple shear [63] and plane stress tension [64] are presented.

3.3 Macroscopic models with microscopic physical roots

The Teodosiu and Hu's hardening model [65-66] is a physically-based microstructural model. Basically, it is able to describe both kinematic and isotropic hardening taking into account the influence of the dislocation structures and their evolutions, at a macroscopic scale. It allows to describe complex hardening behaviours induced by strain-path changes.

The model is described by 13 material parameters and depends on four state variables: $\underline{\underline{P}}, \underline{\underline{S}}, \underline{\underline{\underline{X}}}, R$. The variable $\underline{\underline{P}}$ is a second order-tensor that depicts the polarity of the persistent dislocation structures (PDS) and $\underline{\underline{S}}$ is a fourth-order tensor that describes the directional strength of the PDS's. The scalar R represents the isotropic

hardening due to the randomly distributed dislocations and the second-order tensor $\underline{\underline{X}}$ is the back stress. These state variables evolve with respect to the equivalent plastic strain rate $\dot{p}$ with the form $\dot{Y} = f\ Y\ \dot{p}$. A precise description of these evolution equations can be found in [67]. The yield condition is given by

$$\overline{\sigma} = \sigma_y = Y_0 + R + f\,|\underline{\underline{S}}|\ , \tag{11}$$

where $\overline{\sigma}$ is the equivalent stress, function of $\underline{\underline{\sigma}} - \underline{\underline{X}}$, σ_y is the current elastic limit, Y_0 is the initial size of the yield locus and $R + f\,|\underline{\underline{S}}|$ represents the isotropic hardening. The expression of $\overline{\sigma}$ depends on the definition of the associated yield locus.

For instance, a validation of the Teodosiu and Hu's hardening model coupled with the Minty constitutive law during deep drawing simulations is presented in [68].

Levkovitch and co-workers [69] proposed a similar phenomenological model based on microstructural material behaviour. The evolution of the polarized dislocation structure on the grain level, representing the main cause of the induced flow anisotropy at the macroscopic level is taken into account. Besides the isotropic and kinematic hardening, the model also accounts for the change of the yield locus shape (distortional hardening). The model is validated thanks to metal forming simulations inducing complex strain path changes.

The 3IVM model [54;70] considers three internal variables for the description of the microstructure. These variables are three dislocation type densities: the mobile dislocations, the immobile dislocations in cell walls and the immobile dislocations in cell interiors. This flow stress model is linked to a Taylor-type model in a finite element code to simulate forming processes: stretch forging of an austenitic steel and hot rolling of aluminium alloys are reported in [54].

4 Discussion and future trends

Thanks to the evolution of the computer capabilities, strong progresses have been noticed concerning the multiscale models. Concerning the modelling of the materials anisotropy, three periods can be distinguished.

Before 1900, only a few research teams are involved in this field but clear tendencies are already initiated: the use of Taylor's model with (parallel) computation of the average behaviour of a set of representative crystals or the use of a fitted yield locus formulation based on the initial texture of the material.

Due to a rapid increase of the number of research teams in the polycrystal domain, the period 1990-2000 is characterized by a strong development of sophisticated homogenization techniques in order to supersede the Taylor's model. The first FEM^2

models are proposed so as to take into account texture evolution and adjacent grains interaction. Crystal plasticity finite element method is still rarely developed.

Since 2000, FEM^2 and CPFEM techniques are more and more investigated. Concurrently, the robustness of the texture based yield loci was improved.

Concerning the microstructure modelling, the progress origins are different:
- A better knowledge of the microscopic mechanisms linked to the phase transformations and the recrystallizations yielded to more and more realistic physical models.
- The increasing computation power allows better analyzing dislocation densities associated to different mechanisms, it allows for instance to study the induced microstructure during not only monotonic strain path but also two-stage strain paths[71].

The current evolution of multiscale models concerns the modelling of multiple phase materials (while single phase models were initially developed). Body centred cubic (bcc) and face centred cubic (fcc) material were first investigated because of their rather continuous behaviour. Several models are now devoted to hexagonal closed packed (hcp) lattice material [72,73]. The main complications come from the lower number and the particular orientations of the slip systems (compared to fcc and bcc materials).

The number and the variety of the polycrystalline models rapidly increase. These new models are very helpful for the identification of more simple models. For instance CPFEM models can be used for the validation of micro-macro models.

5 Conclusion

Even without analyzing the atomistic scale, a lot of research work is still required to improve the accuracy of the numerical results compared to the experiment. Several studies concerning forming processes have already been achieved. A lower effort was devoted to the structure toughness and consequently to the fatigue analysis.

The rapidly increasing number of micro-macro research teams prefigures future improvements of the numerical models concerning both their accuracy and their rapidity.

Anyway, the complexity of the numerical model must always be adapted to the material and the process investigated. For instance, if a simple constitutive law (e.g. Von Mises yield locus with isotropic hardening) provides accurate results for the studied process, multiscale models should be avoided. It is important to correctly analyze the complexity of the involved deformation mechanisms in order to choose the most adequate model (multiscale or phenomenological model). Macroscopic phenomenological models based on and identified from micro-macro models should still be taken into consideration as an interesting intermediate solution.

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