

Graphical Abstract

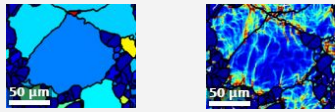
A simplified intragranular description of dislocation density heterogeneities to improve dynamically recrystallized grain size predictions

B. Flipon, N. Bozzolo, M. Bernacki

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Aims and context

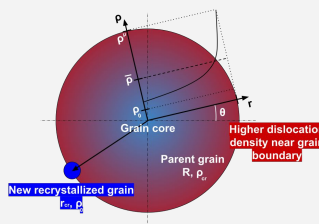
Computational models of dynamically recrystallized grain size predictions are often based on the assumption of a uniform dislocation density distribution within the parent grain.



However, experimental observations show that dislocation density is not uniform, being higher near grain boundaries.

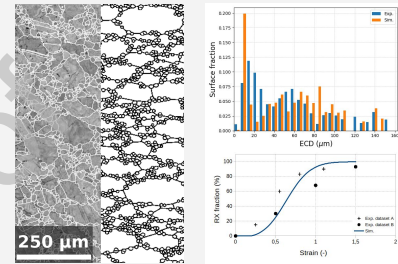
This leads to an overestimation of the grain size, as the model does not account for the higher dislocation density near grain boundaries.

Proposed model



Main results & conclusions

The proposed model shows that the grain size prediction is improved by considering the higher dislocation density near grain boundaries.



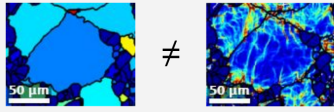
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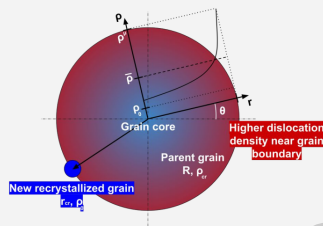
A simplified intragranular description of dislocation density heterogeneities to improve dynamically recrystallized grain size predictions**Aims and context**

Keeping computational costs reasonable in full-field recrystallization models rely on strong hypotheses such as homogeneous dislocation density in grains.



However, experimental observations classically exhibit strong intragranular heterogeneities regarding dislocation density, especially near grain boundaries.

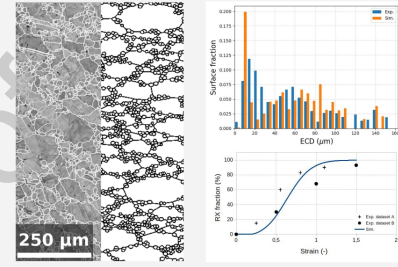
Need to account for intragranular dislocation density heterogeneities while keeping similar computational costs.

Proposed model extension

Improved description of local dislocation density near grain boundaries.

Main results & conclusion

Model extension enables to refine material dependent model parameters which in turn leads to better microstructure evolution predictions.



Symbol	Units	Definition
Model variables		
P		Sum of the driving pressures acting on GB
P_c		GB driving pressure associated to capillarity effects
P_e		GB driving pressure associated to stored energy (due to dislocations)
$\vec{v}$	m.s^{-1}	GB velocity
$\vec{v}_c$	m.s^{-1}	GB velocity due to capillarity effects
$\llbracket E \rrbracket$	J.m^{-3}	Stored energy jump across GB (due to dislocations)
ρ_i	m^{-2}	Average dislocation density of the i^{th} grain
ε		Strain
τ	J.m^{-1}	Energy per unit length of dislocation line
$\dot{\varepsilon}$	s^{-1}	Strain rate
$\Delta\rho$	m^{-2}	Dislocation density difference between a recrystallized grain and its parent grain
Φ	m or m^2	Total length or surface of GBs belonging to grains satisfying the nucleation criterion
Material-dependent model parameters		
M_b	$\text{m}^4.\text{J}^{-1}.\text{s}^{-1}$	GB mobility
M_0	$\text{m}^4.\text{J}^{-1}.\text{s}^{-1}$	Arrhenius law GB mobility pre-exponential factor
Q_m	J.mol^{-1}	Arrhenius law GB mobility apparent activation energy
γ_b	J.m^{-2}	GB energy
δ		Strain rate dependent term for the stored energy driven GB migration
K_1	m^{-2}	Hardening term in the YLJ law
K_2		Recovery term in the YLJ law
K_g	m.s^{-1}	Nucleation probability term depending on processing conditions
Numerical constants		
ω		Numerical factor used to ensure recrystallized grains to grow when they nucleate. Introduced to limit mesh size effect on grain growth following nucleation.

GB stands for Grain Boundary; YLJ for Yoshie-Laasraoui-Jonas.

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ABSTRACT

In current mesoscopic mean-field and full-field models, nucleation of recrystallized grains remains poorly described compared to the physical complexity of the phenomenon, leading to noticeable discrepancy with regards to the size of recrystallized grains. In the present work, a simplified intragranular description of dislocation density heterogeneities is introduced in a recrystallization model in order to improve recrystallized grain size predictions. A detailed material-dependent model parameters identification procedure is provided and discussed. Experimental microstructure evolutions of an Inconel 718 Ni-base superalloy are compared to the model predictions as a validation case.

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1. Introduction

Under hot forming conditions grain growth (GG) and recrystallization (RX) are likely to occur. These phenomena are linked to high temperature and the minimization of energy related to defects present in the material such as grain boundary (GB) interfaces and dislocations stored during plastic deformation. They both impact microstructure evolutions and the final grain size distribution of the material. As (mean) grain size (GS) is directly related to the material mechanical properties [17, 38], microstructure control along the process is often necessary depending on the targeted use of the material.

Since the seminal works of Kolmogorov and Avrami [23, 3, 21] in the late 1930's and further modifications leading to the so-called Johnson-Mehl-Avrami-Kolmogorov (JMAK) analytical model, different modeling strategies have been developed. These approaches rely either on modified versions of the JMAK equation, on mean field models [31, 8, 6, 48, 27] or on models with an explicit representation of the microstructure and its evolutions [19]. In the latter full-field framework, several formalisms can be used, such as: Monte-Carlo [41, 36], cellular automata [39, 25], phase-field [10], vertex [5], front-tracking [14], or level-set [7, 18, 44, 28]. These methods have a high computational cost compared to mean field modeling and JMAK predictions but they proved to be able to provide an accurate tracking of microstructural variations during the process [28] and are also able to account for topological heterogeneities.

While grain boundary migration can be described by full-field modeling, strain hardening and associated dislocation density evolution are often described by phenomenological laws to keep computational costs reasonable. More physical formulations may be used such as crystal plasticity [12, 43] at the expense of additional computation costs. One of the main limitations using phenomenological laws is that only grain averaged [28] or grain boundary averaged [20] responses of the polycrystal are available. The latter may be limiting in some models, for example when recrystallized grain size is directly proportional to a dislocation density value [4]. To circumvent this limitation, a simplified intragranular description of dislocation density heterogeneities is proposed in this work in order to improve recrystallized grain size predictions.

After a detailed presentation of the numerical framework and particularly of the equations used to model grain boundary migration, hardening, recovery and nucleation, a scaling equation between local dislocation density values and grain averaged ones is introduced. The motivation and the experimentally-driven origins of this modified model are detailed in a separate section. An applicative case is then proposed for the sake of validation. For each mechanism, the material-dependent parameters identification is explained (and detailed in appendix A for hardening/recovery and dynamic recrystallization parameters) and illustrated with experimental data. This identified set of parameters for the Inconel 718 Ni-based superalloy is then used and simulation results are confronted to experimental observations. Conclusions and perspectives are finally drawn regarding the modified model and its influence on the predicted results.

2. Numerical framework

2.1. A full-field level-set approach

The full-field results presented in this work are obtained within the finite element level-set framework of the DIGIMU[®] software. Each grain boundary is explicitly represented and tracked during simulation by a level-set function. If a domain Ω is considered, the position of a grain boundary Γ will be described by a level-set function ψ by considering:

$$\begin{aligned}\psi(\underline{x}) &= d(\underline{x}, \Gamma), \quad \underline{x} \in \Omega \\ \Gamma &= \{\underline{x} \in \Omega, \psi(\underline{x}) = 0\}\end{aligned}\tag{1}$$

$\underline{x}$ being the coordinates of a point belonging to Ω .

The grain boundary is defined by the 0 iso-value of the level-set function which is defined positive ($\psi > 0$) inside the considered grain and negative ($\psi < 0$) outside.

To limit computation costs, improvements have been made regarding the number of level-set functions used to describe a polycrystal [44], remeshing [7] and level-set numerical treatment (reinitialization) [46]. More details can be

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found in [7, 44, 28] about finite element level-set modeling of grain growth and/or recrystallization. Figure 1 provides an illustration of the capabilities of the DIGIMU[®] model: after hot deformation inducing discontinuous dynamic recrystallization (DDR), a high temperature holding is performed during which post-dynamic microstructure evolutions occur.

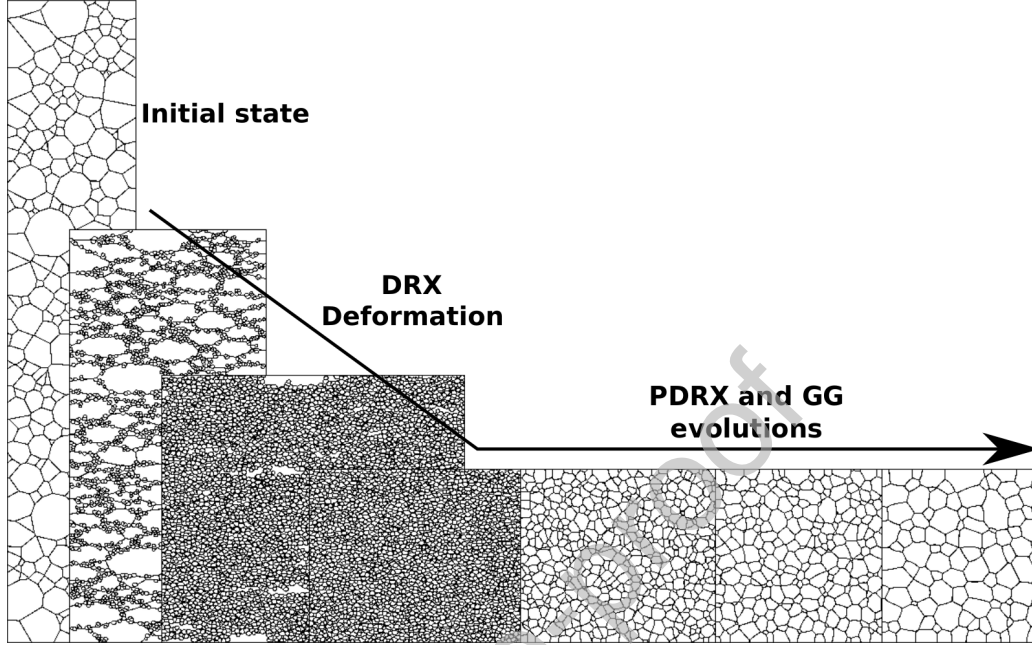


Figure 1: 2D simulation performed using the DIGIMU[®] software of a hot deformation (DDR) followed by a subsequent holding at high temperature (post-dynamic evolutions).

2.2. Current model and equations used in the DIGIMU[®] software

The model is constructed around blocks, each one being associated to a specific mechanism. The following sections will describe the equations associated to grain boundary migration, dynamic hardening and recovery and recrystallization.

2.2.1. Grain boundary migration

In a single-phase material and during conventional thermomechanical treatment, the grain boundary migration is driven by two distinct driving pressures:

1. Grain boundary energy considerations which result in curvature-driven GB migration linked to capillarity effects.
2. Influence of grain to grain difference in stored energy due to plastic deformation anisotropy.

When ψ remains a distance function ($\|\vec{\nabla}\psi\| = 1$), the unitary outside normal of the corresponding GBs can be evaluated as $-\vec{\nabla}\psi$ and the curvature as $-\Delta\psi$ (following the sign level-set convention described previously). As a result, GB migration can be described by the following set of equations in the DIGIMU[®] level-set framework:

$$P = P_c + P_e, \quad (2)$$

$$P_c = -\gamma_b \kappa, \quad (3)$$

$$P_e = \delta[E], \quad (4)$$

$$\vec{v} = M_b P \vec{n}, \quad (5)$$

$$\vec{v} = -M_b (\gamma_b \Delta\psi + \delta[E]) \vec{\nabla}\psi. \quad (6)$$

The strain rate dependent term δ in eq. (4), has been added to the initial formulation proposed by Beltran *et al.* [6]. It enables to separate the influence of temperature (taken into account through the mobility term $M_b(T)$) from that of

A simplified intragranular description of dislocation density heterogeneities to improve DRX grain size predictions the strain rate (with $\delta(\dot{\epsilon})$) for the description of the GB migration during a dynamic regime [26].

In the case of curvature-driven GG:

- The material is considered free of dislocations, *i.e.* the material is in a fully recrystallized state and is free of any residual stored energy due to previous deformation history which means that $P_e = 0 \text{ J.m}^3$.
- The GB migration is only related to a curvature flow problem minimizing the GB network energy.

Therefore, the only remaining material-dependent parameters are M_b and γ_b within the GB velocity equation:

$$\vec{v} = \vec{v}_c = -M_b \gamma_b \Delta \psi \vec{\nabla} \psi. \quad (7)$$

γ_b values can be found for most materials in literature and the evolution of M_b as a function of temperature can, usually, be modeled by a Arrhenius law :

$$M_b = M_0 \exp\left(\frac{-Q_m}{RT}\right), \quad (8)$$

which implies to determine the values of the pre-exponential factor M_0 and of the activation energy for grain boundary migration Q_m .

2.2.2. Work hardening and dynamic recovery

The current model used in the DIGIMU[®] framework relies on the dislocation density as an internal variable in order to describe discontinuous dynamic recrystallization kinetics.

Hardening and recovery are described by a phenomenological law based on the works of Yoshie-Laasraoui-Jonas (YLJ) [50, 24]. Physically, strain hardening is linked to the formation, multiplication, entanglement and pile-up of dislocations in the material. Recovery is promoted by high temperatures and consists in dislocation annihilation and the formation of intragranular substructures. The YLJ law (eq. (9)) links the evolution of dislocation density with strain through two material-dependent parameters: K_1 and K_2 being associated with hardening and recovery, respectively. While the original YLJ law has been proposed to describe the macroscopic hardening and recovery of a polycrystal, in DIGIMU[®] it is used at the scale of each grain (see eq. (10)).

$$\frac{\partial \rho}{\partial \epsilon} = K_1 - K_2 \rho, \quad (9)$$

$$\frac{\partial \rho_i}{\partial \epsilon} = K_1 - K_2 \rho_i, \quad (10)$$

with ρ and ρ_i the average dislocation density of the polycrystal and the i^{th} grain, respectively, and ϵ the strain.

Dislocation density per grain ρ_i can be used to obtain the average stress per grain σ_i through the Taylor equation [49]:

$$\sigma_i = \sigma_0 + M_T \alpha \mu b \sqrt{\rho_i}. \quad (11)$$

The mean flow stress value σ is finally obtained by an area (in 2D; resp. volume in 3D) weighted average.

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2.2.3. Nucleation of recrystallized grains

The critical dislocation density used in DIGIMU[®] as a nucleation criterion is derived from the work of Roberts and Ahlblom [40]. This criterion relies on the Bailey-Hirsch bulge mechanism [4] which considers that nucleation occurs preferentially at existing grain boundaries.

The critical dislocation density ρ_{cr} is first initialized:

$$\rho_{cr} = \left(\frac{20K_1\gamma_b\dot{\epsilon}}{3M_b\delta\tau^2} \right)^{1/3}, \quad (12)$$

and then an iterative solution can be computed:

$$\rho_{cr} = \left[\frac{-\gamma_b\dot{\epsilon}\frac{K_2}{M_b\delta\tau^2}}{\ln\left(1 - \frac{K_2}{K_1}\rho_{cr}\right)} \right]^{1/2}. \quad (13)$$

The critical recrystallized grain size is linked to the Bailey-Hirsch criterion and associated with the dislocation density difference $\Delta\rho$ between the new recrystallized grain and its strain-hardened parent grain:

$$D_{cr} = 2 \times R_{cr} = 2 \times \omega \frac{\gamma_b}{\tau\Delta\rho}. \quad (14)$$

If ρ_0 is negligible compared to ρ_{cr} , then $\Delta\rho = \rho_{cr}$; if not $\Delta\rho = (\rho_{cr} - \rho_0)$. The constant ω is a numerical security factor linked to finite element mesh issues that can occur if the recrystallized grain is too small compared to the mesh size. It should be seen as a safety factor ensuring recrystallized grains to grow and not disappear by numerical diffusion. It is taken here equal to 1.5 as in previous works [28, 27]. Implementation wise, eq. (14) is rewritten as:

$$D_{cr} = 2 \times \omega \frac{\gamma_b}{\tau \max(\bar{\rho}, \rho_{cr})}. \quad (15)$$

ρ_0 is considered negligible compared to ρ_{cr} and if the mean dislocation density $\bar{\rho}$ is higher than ρ_{cr} then $\bar{\rho}$ is used instead of ρ_{cr} to obtain D_{cr} .

In the model, K_1 and K_2 are used to calculate the critical dislocation density (through eqs. (12) and (13)) needed to trigger nucleation of recrystallized grains and their associated critical grain size D_{cr} (eq. (14)). The identification of K_1 and K_2 values will then also have an influence on the nucleation criterion and on the recrystallization kinetics.

The nucleation rate (*i.e.* nucleation volume per time step) is calculated based on the model proposed by Peczak and Luton [37]:

$$\dot{V}_{nucl} = K_g \Phi, \quad (16)$$

with K_g a nucleation probability term associated with the considered thermomechanical conditions and Φ the total length (in 2D) or area (in 3D) of grain boundaries belonging to grains satisfying $\rho_i \geq \rho_{cr}$.

2.2.4. Post-dynamic microstructure evolutions

In this work only meta-dynamic evolutions are considered within the post-dynamic regime. Only static recovery and grain growth can occur in this case.

Static recovery is supposed to be of secondary importance compared to stored energy reduction associated with grain boundary migration. In the following eq. (17), K_s is similar to the dynamic parameter K_2 but is here considered equal to 0.

$$\frac{\partial \rho}{\partial t} = -K_s \rho, \quad (17)$$

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The only source of energy reduction is then coming from grain boundary migration due to stored energy in grains and capillarity effects (eq. (6)). In the present case no specific identification is necessary for post-dynamic evolutions considering only meta-dynamic recrystallization and no static recovery. This explains why no specific subsection will be dedicated to post-dynamic model parameters identification in section 4.2.

3. Introduction of a simplified description of intragranular dislocation density heterogeneities

3.1. Why considering intragranular dislocation density heterogeneities ?

As already stated by Burke and Turnbull in their seminal work in 1952 [9] (p. 243):

"It is significant that recrystallized grains do not originate at random in a strained matrix but preferentially at intersecting slip lines, strain markings, twin boundaries and often at a free surface, edges or grain boundaries. [...] These preferential nucleation sites are generally supposed to be regions in which the stress is much higher than in the surrounding matrix."

As described by Burke and Turnbull, physically, dislocation densities are heterogeneous over a grain. Experimentally it can be seen using EBSD data and local misorientations analysis that provides an insight of the geometrically necessary dislocation (GND) density field. More details on this aspect may be found in experimentally focused works such as in ref. [35, 47, 45]. As an example, fig. 2 provides a GND map obtained by processing of EBSD data of a partially recrystallized Inconel 718 sample, using the method described in ref. [35].

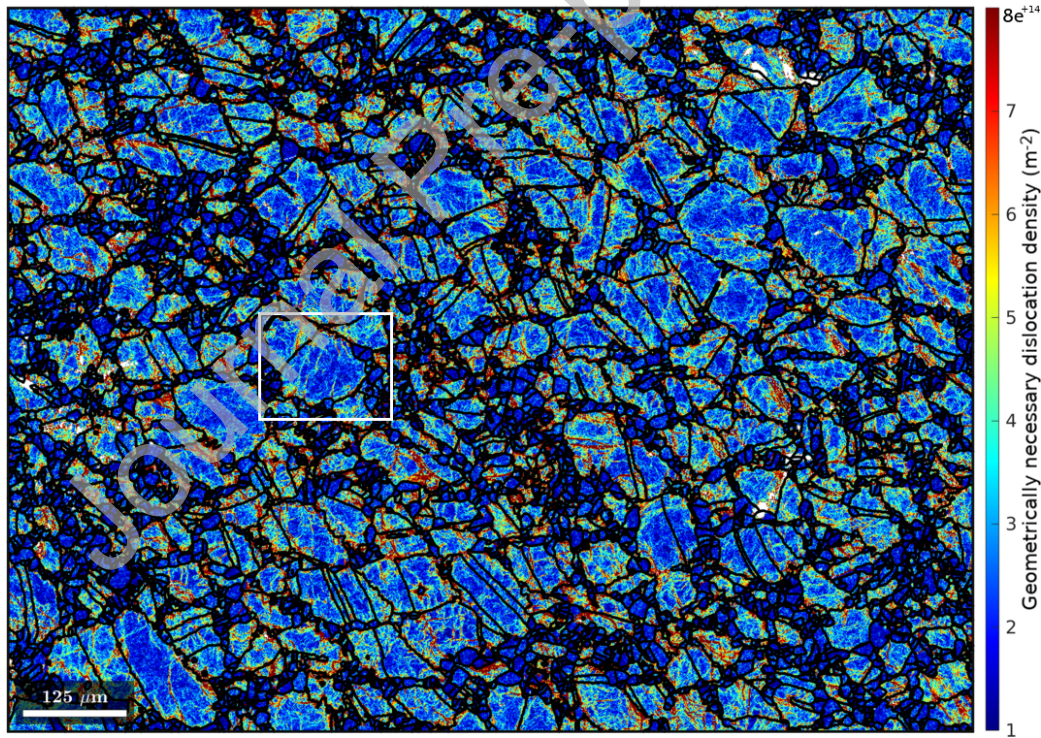


Figure 2: Experimental GND map obtained by processing EBSD data. Inconel 718 sample after a hot deformation at 1050°C at 0.1 s⁻¹ and a strain level of 0.5.

Areas near to GBs are expected to concentrate GNDs due to deformation incompatibilities between the neighboring grains [2] and are also favourable areas for dislocation piling-up. Heterogeneities might also develop inside grains, as dislocation cells or veins form during deformation [29] or near twin boundaries. To precisely account for intragranular heterogeneities regarding dislocation density, crystal plasticity may be used [43, 42] but at the expense of a higher computational cost. In order to accurately describe twin boundaries, GB anisotropy has to be taken into account in

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terms of misorientation but also for the inclination [11, 33, 13] which requires complex experimental analyses (e.g. 3D EBSD). The fact to take into account torque terms in the FE formulation [14] also leads to a higher computational cost. Until further improvements of the used full-field numerical formalism, these aspects were not included in the proposed model described in the following section.

3.2. Proposed model to account for higher dislocation densities near to GBs

In most of the grains of fig. 2 and better visible in the zoomed example in fig. 3, the dislocation density differs from the grain core to regions close to grain boundaries. Regions near GBs should accommodate strain incompatibilities arising from neighboring grains with the creation of geometrically necessary dislocations [2] and dislocation piling-up during deformation.

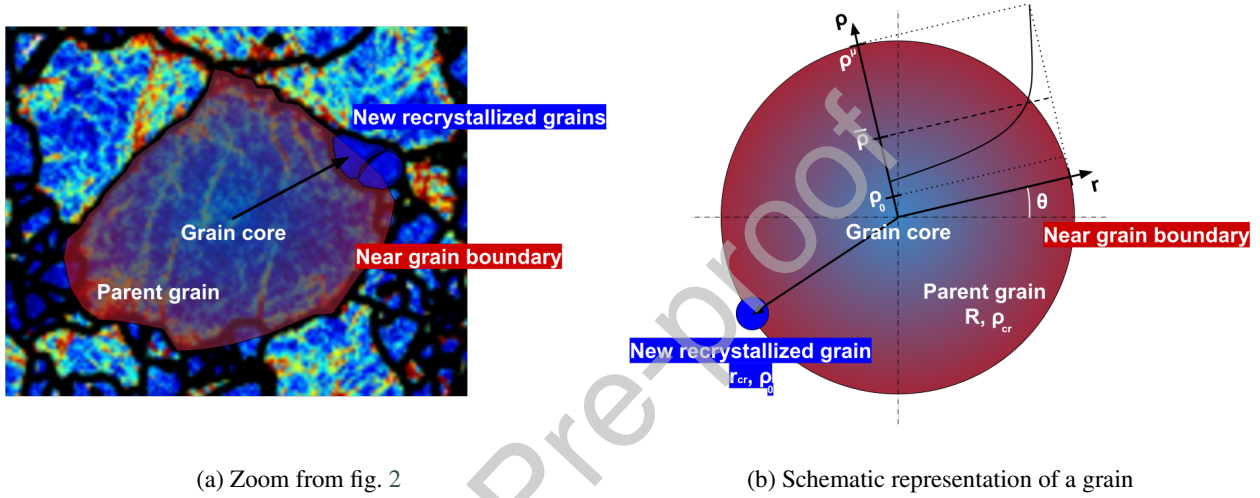


Figure 3: Experimental and schematic description of GND heterogeneities over a grain.

Two different hardening behaviors are expected in these two regions. The region close to the GB is expected to harden faster and store higher GND densities than the grain core. This should, in turn, result in heterogeneous GND dislocation density with higher values close to GB and lower ones in the grain core. One may notice that intragranular heterogeneities arise also along slip lines in the grain interior on the experimental microstructure (cf. fig. 3a). Since only nucleation at existing GBs is considered in the model, the simplified representation of fig. 3b will be used in the following developments.

In the proposed model, the dislocation density is distributed along the radius of the grain with the highest value near grain boundary and the lowest at the grain core as shown on fig. 3b. In the following ρ^μ is associated to the local hardening behavior (that will be used to obtain ρ_{cr} and D_{cr}) near the GB. The hardening and recovery material parameters of the YLJ law are set to describe the local hardening and are denoted accordingly (K_1^μ , K_2^μ). In order to obtain the mean dislocation density of the whole grain, and in turn of the whole polycrystal, a homogenization strategy at the grain scale has to be chosen.

We impose a general expression for the ρ distribution along the radius ($\rho(r)$) with a power law leading to a profile as drawn in fig. 3b:

$$\rho(r) = c \times \left(\frac{r}{R}\right)^n, \quad (18)$$

c being a constant and R the grain radius. n is a constant (tunable exponent) assumed to be dependent on the material but not on the thermomechanical conditions (i.e. temperature and strain rate).

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The expression of c is derived on the basis of mean dislocation density conservation in each grain, *i.e.* the area under the curve considering a constant mean value of ρ along the radius (see the dashed line in fig. 3b) should be the same than the one considering a particular distribution of ρ along the radius (the assumed power law in solid line in fig. 3b):

$$\begin{aligned} \int_{\text{Grain}} \bar{\rho} dS &= \int_{\text{Grain}} c \times \left(\frac{r}{R}\right)^n dS, \\ \int_0^{2\pi} \int_0^R \bar{\rho} r dr d\theta &= c \int_0^{2\pi} \int_0^R \left(\frac{r}{R}\right)^n r dr d\theta, \\ \bar{\rho} \pi R^2 &= c \frac{2}{n+2} \pi R^2, \\ c &= \bar{\rho} \frac{n+2}{2}. \end{aligned} \quad (19)$$

Then replacing c in eq. 18, it comes:

$$\rho(r) = \bar{\rho} \frac{n+2}{2} \times \left(\frac{r}{R}\right)^n, \quad (20)$$

which enables to link the dislocation density near GB to the mean dislocation density of a given grain:

$$\rho^\mu = \rho(R) = \bar{\rho} \frac{n+2}{2}. \quad (21)$$

Experimentally only the global hardening behavior of the material (through stress-strain curves) is available using classical mechanical tests. For identification purposes, the scaling equation eq. (21) is rewritten as follows in order to retrieve the average dislocation density per grain:

$$\rho_i = \left(\frac{2}{n+2}\right) \rho_i^\mu, \quad (22)$$

Eq. (22) is then used in the Taylor equation (11) to obtain the average stress per grain σ_i and mean flow stress is then still computed based on an area (in 2D) or volume (in 3D) weighted average.

4. Applicative case: Hot deformation of Inconel 718

All simulations presented in this section are realized in 2D in order to limit the computational cost compared to 3D simulations. Material-dependent model parameters are identified based on microstructural 2D experimental data. Comparisons between 2D polycrystals and 2D experimental cross-sections are provided in the validation part associated to dataset C.

4.1. Experimental plan and data

Datasets A and B are used for the parameters identification (GG and DRX data extracted from Zouari *et al.* [52, 51]). Dataset C (previously unpublished data) is then used as a validation case for the identified parameters over a complete range of mechanisms including GG, DRX and post-dynamic evolutions. All heat treatments and holding at temperature were done using a conventional resistive furnace. All hot deformation tests were performed in torsion. Table 1 summarizes all the experimental points used in this work. For each deformation condition, the Zener-Hollomon parameter $Z (= \dot{\epsilon} \exp(\frac{Q_{def}}{RT}))$ is computed using the apparent activation energy $Q_{def} = 4 \times 10^5 \text{ J.mol}^{-1}$ [30]. Figure 4 illustrates the thermomechanical paths of each dataset.

For all the experimental results presented in this work, D (and $R = D/2$) or ECD all refer to the same definition of the mean grain size being the Equivalent Circle Diameter (ECD). The latter is defined as the diameter of the circle whose area is the one of the considered grain measured in a 2D section. It should be noted that *mean* value is meant here as an arithmetic average value. Experimental EBSD maps used in section 4.3.3 (Dataset C) are acquired over the area schematically represented in figure 5. This area is located on a narrow section 2 mm wide and 10 mm long, its longitudinal direction (LD) being parallel to the sample rotation axis. EBSD acquisition conditions are similar to

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Test	Mechanism	Conditions	Z	Source
A1	GG	$T = 1020^{\circ}\text{C}$ for $t = 3600$ s		[51]
A2	GG	$T = 1035^{\circ}\text{C}$ for $t = 3600$ s		[51]
A3	GG	$T = 1050^{\circ}\text{C}$ for $t = 3600$ s		[51]
A4	GG	$T = 1080^{\circ}\text{C}$ for $t = 3600$ s		[51]
B1	DRX	$T = 1000^{\circ}\text{C} - \dot{\epsilon} = 0.03 \text{ s}^{-1}$	7.7×10^{14}	[52, 51]
B2	DRX	$T = 1010^{\circ}\text{C} - \dot{\epsilon} = 0.05 \text{ s}^{-1}$	9.6×10^{14}	[51]
B3	DRX	$T = 1020^{\circ}\text{C} - \dot{\epsilon} = 0.1 \text{ s}^{-1}$	1.4×10^{15}	[51]
B4	DRX	$T = 1030^{\circ}\text{C} - \dot{\epsilon} = 0.05 \text{ s}^{-1}$	5.4×10^{14}	[51]
B5	DRX	$T = 1040^{\circ}\text{C} - \dot{\epsilon} = 0.05 \text{ s}^{-1}$	4.1×10^{14}	[51]
B6	DRX	$T = 1050^{\circ}\text{C} - \dot{\epsilon} = 0.1 \text{ s}^{-1}$	6.2×10^{14}	[51]
C1	GG	$T = 1050^{\circ}\text{C}$ for $t = 300$ s		this work
C2	DRX	$T = 1050^{\circ}\text{C} - \dot{\epsilon} = 0.1 \text{ s}^{-1}$	6.2×10^{14}	this work
C3	Post-dynamic evolutions	$T = 1050^{\circ}\text{C}$ for $t = 600$ s		this work

Table 1

Experimental points used in this work.

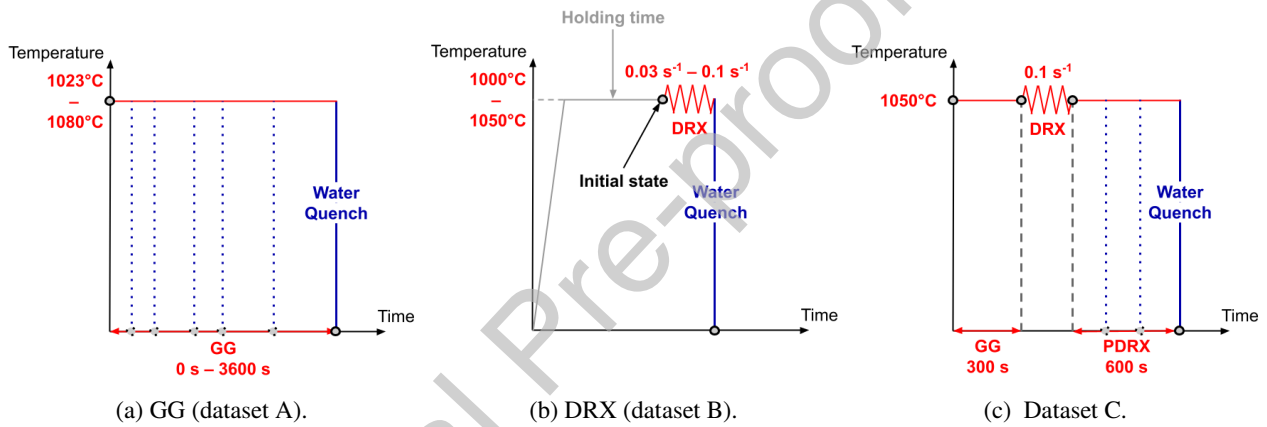


Figure 4: Thermomechanical paths for the different datasets given in table 1.

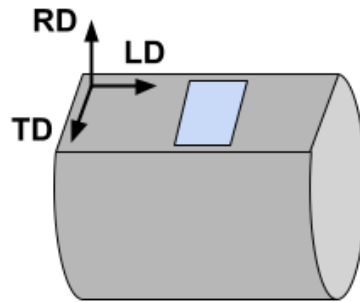


Figure 5: Observation area on torsion samples.

those used by Zouari *et al.* [51]. Grains are detected using a 5° misorientation angle threshold and their area has to be comprised of 3 and 10 pixels for dataset B [51] and C, respectively. Since twin boundaries ($\Sigma 3$) are not modeled in the used DIGIMU[®] framework (v4.6), they are also filtered out from experimental EBSD maps and thus not taken into account in grain size measurements. Numerically, the mean grain size is define as the average ECD of the grains of the

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polycrystal.

As detailed in ref. [51], experimental recrystallized grains and recrystallized fraction can be defined using either a grain size or a intragranular misorientation threshold below which a grain is considered as recrystallized. The Grain Orientation Spread (GOS) and the Kernel Average Misorientation (KAM) are two of the common parameters used to quantify intragranular misorientation based on EBSD maps and are usually used to distinguish recrystallized grains from deformed ones in the microstructure. Experimentally, the recrystallized fraction is thus *the area fraction of the 2D EBSD map occupied by the grains satisfying the applied criterion for RX grains detection*. Numerically, recrystallized fraction is defined as the area or volume fraction corresponding to *all the grains that have appeared/nucleated during the simulation*. Alternatively, a maximum grain size threshold may also be used in the analysis of numerical results. It should also be noted that, numerically, grains with a very small size are also considered when evaluating a mean RX grain size.

4.2. Material-dependent model parameters identification

4.2.1. Grain growth model parameters

Figure 6a illustrates the experimental points (from ref. [51]) alongside simulation results after model parameters refinement for grain growth of Inconel 718.

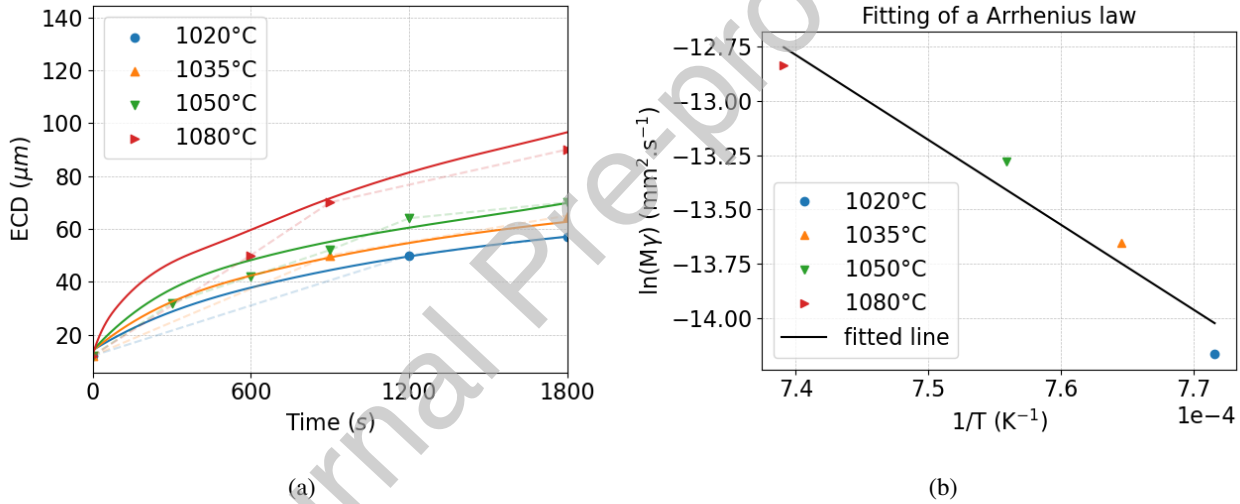


Figure 6: Grain growth parameters identification. (a) Experimental points (from ref. [51] - dataset A) and simulation results after model parameters refinement and (b) Arrhenius law describing $M_b(T)$.

Grain growth material-dependent model parameters, M_0 , Q_m and γ_b (eq. (8)), have been identified using the following procedure:

1. the reduced GB mobility ($M_b\gamma_b$ product) is estimated using the Burke & Turnbull law (eq. (23)).

$$\bar{R}^2 - \bar{R}_0^2 = \frac{1}{2} M_b \gamma_b t, \quad (23)$$

$\bar{R}$ and $\bar{R}_0$ being the mean grain radius (ECD/2) and the initial mean grain radius, respectively, and t the time.

2. a first DIGIMU[®] simulation is launched using this value of $M_b\gamma_b$.
3. results of this first simulation are compared to experimental points and the L^2 error is minimized between experimental data and simulation results.
4. a new value of $M_b\gamma_b$ is obtained after step 3 fit.

This procedure is repeated for each temperature of the experimental dataset in order to obtain fitted values of $M_b\gamma_b$ for all temperatures. γ_b is considered isotropic and constant and is taken from literature [16] (here GB energy of

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M_0	Q_m	γ_b
$\text{m}^4 \cdot \text{J}^{-1} \cdot \text{s}^{-1}$	$\text{J} \cdot \text{mol}^{-1}$	$\text{J} \cdot \text{m}^{-2}$
17.915	325560	0.6

Table 2

Inconel 718 grain growth material parameters.

	Temperature					
	1000°C	1010°C	1020°C	1030°C	1040°C	1050°C
$\dot{\epsilon}$	0.01 s ⁻¹					
	0.03 s ⁻¹	σ - ϵ ; RX				
	0.05 s ⁻¹		σ - ϵ ; RX	σ - ϵ	σ - ϵ ; RX	
	0.1 s ⁻¹		σ - ϵ ; RX			RX

Table 3

Complete thermomechanical conditions matrix. Experimental data availability for material parameters identification are indicated by σ - ϵ for stress-strain curves and RX for RX fraction and RX mean grain size. Temperature range: 1000°C – 1050°C; strain rate range: 0.01 s⁻¹ – 0.1 s⁻¹.

pure Ni). The evolution of M_b with respect to temperature is then obtain through a Arrhenius law with M_0 and Q_m parameters (see fig. 6b). Grain growth model parameters for Inconel 718 are given in table 2.

A similar procedure has been used by Alvarado *et al.* [1] and by Murgas *et al.* [32]. The procedure providing each time good results in terms of mean grain size and grain size distribution evolution predictions.

4.2.2. Dynamic recrystallization model parameters

Dynamic recrystallization parameters are obtained applying the identification procedure detailed in appendix A and the model extension to account for intragranular heterogeneous dislocation density presented in subsection 3.2.

The data available in ref. [52, 51] are scarce but the dataset was designed taking into account the Zener-Hollomon parameter Z . Each thermomechanical condition has its own Z value (see table 1): this approach may be used in order to limit the number of tests for material parameters identification. It is worth noting that temperatures and strain rates remain close to each other in this dataset which in turn make it possible to only use this limited number of points for identification.

Table 3 presents the experimental matrix available for DRX parameters identification. Material parameters values for the other thermomechanical conditions of the table have been obtained by interpolation or slight extrapolation (*e.g.* for $\dot{\epsilon} = 0.01 \text{ s}^{-1}$) using the following mathematical equations.

$$K_1^\mu = 6.49 \times 10^3 \times Z^{0.76}, \quad (24)$$

$$K_2^\mu = 3.17 \times 10^{-4} \times Z^{0.29}, \quad (25)$$

$$K_g = 3.04 \times 10^{-48} \times T^{16.05} \times \dot{\epsilon}, \quad (26)$$

$$\delta = 1.03 \times \exp(17.19 \times \dot{\epsilon}). \quad (27)$$

4.3. Full-field simulation results

4.3.1. Comparing homogeneous average dislocation density per grain and heterogeneous intragranular dislocation density

To compare the impact of an average dislocation density per grain vs. an heterogeneous one, a single thermomechanical condition is considered: $T = 1040^\circ \text{C}$ and $\dot{\epsilon} = 0.05 \text{ s}^{-1}$ (lowest Z of the dataset B).

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Considering a homogeneous average dislocation density per grain A first approach may be to only consider the average mechanical behavior of the material (or polycrystal) using macroscopic stress-strain curves [22, 26]. In eq. (22), this is equivalent to consider $n = 0$. In this case, the YLJ law provides the evolution of the mean dislocation density of the material since K_1 and K_2 are identified solely based on the experimental macroscopic stress-strain curve. This will provide accurate predictions of the macroscopic mechanical behavior but will not necessarily be suitable for microstructure predictions. Figure 7a illustrates the stress-strain curve obtained with a macroscopic evaluation of K_1 and K_2 as proposed by Jonas *et al.* [22].

As a reminder, in the present model, the size of a new recrystallized grain to be introduced is computed based on the Bailey-Hirsch criterion (eq. (14)) which relies on the equilibrium between capillarity and energy-driven forces acting on the grain boundary of the new recrystallized grain with respect to its environment (= its parent grain). As stated in section 2.2.3, considering $\rho_0 \ll \rho_{cr}$, D_{cr} is inversely proportional to ρ_{cr} .

ρ_{cr} is calculated using eq. (12) and eq. (13). Considering the model parameter values for Inconel 718 and the macroscopic K_1 and K_2 parameters identified, ρ_{cr} is about $1.6 \times 10^{13} \text{ m}^{-2}$ leading to an associated recrystallized grain diameter (eq. (14)) of about $75 \text{ }\mu\text{m}$. This value is much larger than typical size of physical RX grain nuclei and larger than the measured RX grain size ($\approx 5 \text{ }\mu\text{m}$).

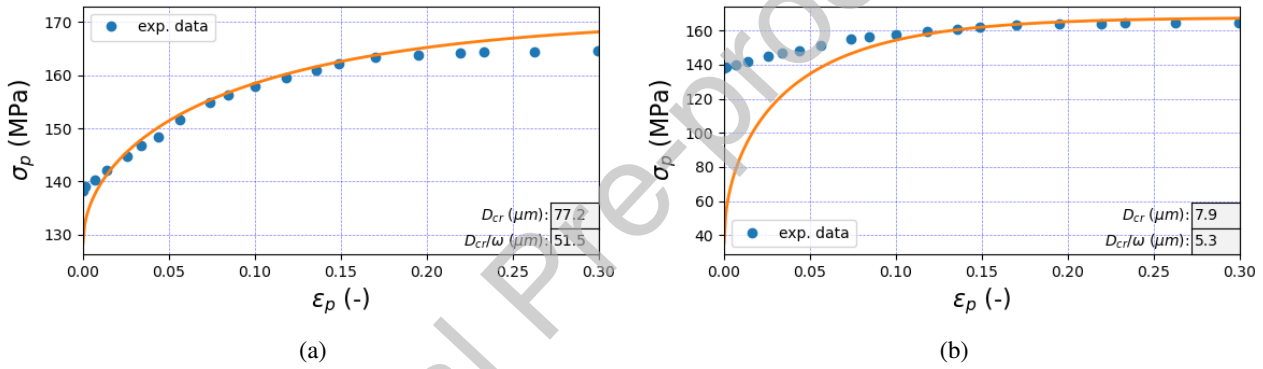


Figure 7: Yoshie-Laasraoui-Jonas model fitted (a) solely on the macroscopic stress-strain curve and (b) with respect to both stress-strain curve and recrystallized grain diameter. The p -subscript stands for *plastic*.

In order to obtain more consistent RX grain sizes (wrt experimental values), the hardening/recovery model parameters (K_1 , K_2) should be modified. By increasing K_1 , ρ_{cr} is higher which results in smaller D_{cr} values. Increasing K_1 implies to modify also K_2 and σ_0 to match the model at least partly with the curve. Fig. 7b illustrates the result: the mechanical response (especially at the beginning of the curve) is clearly deviating from the experimental macroscopic one.

Considering a heterogeneous intragranular dislocation density As introduced in section 3.2, the n parameter is used to account for hardening differences between the core and near GB areas in a grain: dislocation density is not anymore homogeneously described in a grain but evolves along grain radius. The YLJ law is associated with the dislocation density near GB and eq. (22) is used to obtain the mean dislocation density over a grain. The latter being used in the Taylor equation (eq. (11)) to link dislocation density to stress in the polycrystal which enables to plot the stress-strain curve presented in fig. 8. The core of the identification procedure remains similar to the one used previously and detailed in appendix A. K_1 and K_2 are now denoted K_1'' and K_2'' since they represent the local, near grain boundary, dynamic hardening and recovery. To get the results shown in fig. 8 the n parameter has been identified for Inconel 718 and is taken equal to 16. Considering a more physical spatial distribution of intragranular dislocations enables both a better description of macroscopic mechanical response and of predicted recrystallized grain size. The predicted RX grain size is now about $8 \text{ }\mu\text{m}$, much closer to the experimental value.

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Even if the n parameter value can be evaluated on stress-strain curves only, here the value of 16 is also coherent with the GNDs map scale presented in fig. 2. For this particular case, ρ_{GND} varies from about 1×10^{14} to 8×10^{14} . In areas where ρ_{GND} is the highest, it is at least 8 times higher than in areas with low ρ_{GND} . In our model, taking a value of $n = 16$ results in dislocation density 9 times higher close to GBs than the mean dislocation density which is close to what can be estimated experimentally.

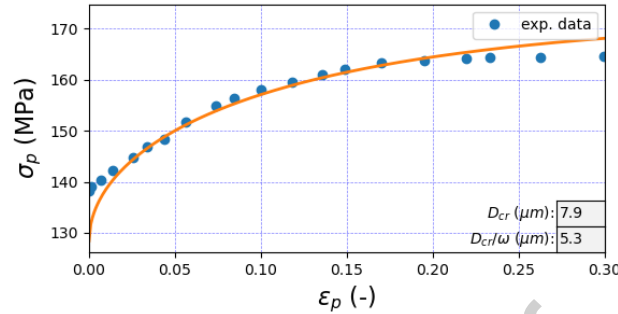


Figure 8: Local Yoshie-Laasraoui-Jonas model associated to scaling equation (22) fitted on macroscopic stress-strain curve and recrystallized grain size. The p -subscript stands for *plastic*.

4.3.2. Identification results obtained on datasets A and B

Initial 2D microstructures for full-field simulations are generated using lognormal distributions with mean and standard deviation coming from experimental data. The initial number of grains (and thus the domain size) depends on the initial mean grain size and on the considered mechanism. For GG / dataset A, 8000 grains have been used and 300 grains for DRX / dataset B. The low initial number of grains for DRX simulations is explained by the fact that RX grains will nucleate during the deformation hence causing a rapid increase of the number of grains in the domain.

Results in terms of recrystallized fraction evolution and stress-strain curves for dataset B are provided in figures 9 and 10, respectively. In each case a good agreement is observed between available experimental points and simulation results. Fig. 11 provides a comparison between the experimental and predicted recrystallized grain sizes. D_{rx} is the evolution of the mean recrystallized grain size with increasing strain. The latter is computed based on a grain size threshold equal to $2 \times D_{cr}$ (obtained with eq. (14)).

Results are all in good agreement with experimental points which proves the proposed identification procedure with the intragranular dislocation density model extension to work for Inconel 718 for the considered (T, ϵ) range.

4.3.3. Validation results obtained on dataset C

Further validation of the procedure / model extension and of the identified parameters is proposed in this section. A thermomechanical path involving grain growth, dynamic and post-dynamic evolutions is simulated and results are compared to experimental data. Material is still Inconel 718 superalloy but the manufacturer differs from the one of datasets A and B. Initial microstructures for dataset C simulations are also generated using lognormal distributions with mean and standard deviation coming from experimental data. 4000 initial grains are used for the GG simulation while for similar reasons to dataset B, only 300 initial grains are considered for DRX and post-dynamic conditions.

Figure 12 presents the RX kinetic and the evolution of the mean grain size predicted during the thermomechanical path of fig. 4c. Both results are in quite good agreement compared to experimental points.

Figures 13, 14 and 15 present qualitative and quantitative comparisons of, respectively, microstructure and grain size distribution evolutions through GG, DRX and post-dynamic evolutions steps of dataset C. Overall predictions are close to experimental EBSD maps and grain size distributions. Predicted grain size distributions during DRX are narrower than experimental ones. This can be explained by the fact that in the model every recrystallized grain appears with the same size (based on the Bailey-Hirsch criterion – eq. (14)). The latter implying a narrowing of the grain size distribution around this mean recrystallized grain size value during DRX. Experimentally, it exists more local

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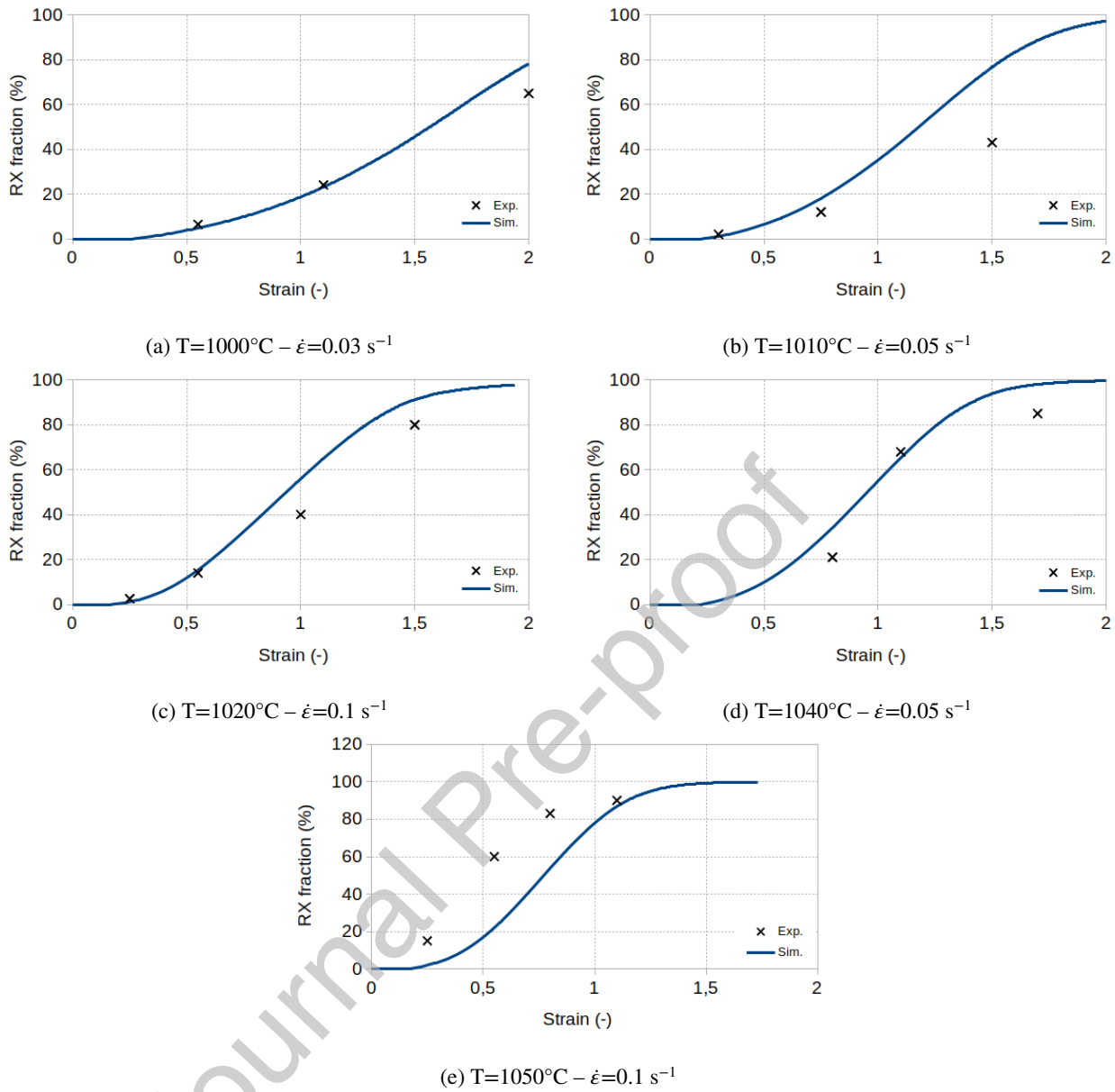


Figure 9: Recrystallized fraction evolution with respect to strain level for dataset B.

heterogeneities which leads to a broader grain size distribution: recrystallization is happening more heterogeneously in the microstructure and recrystallized grains may evolve more or less quickly depending on their specific neighborhood. The fact to only consider an isotropic grain boundary mobility/energy for all grains in the microstructure may also explain a more uniform microstructure evolution by simulation than in reality. During the post-dynamic regime grain boundary migration tends to broaden again grain size distributions which is correctly captured by the model up to 300 s. After a 600 s holding at 1050°C , the predicted mean grain size is smaller than the experimental one which may be imputed, once again, to the more homogeneous energy gradients in the numerical microstructure than experimentally.

5. Conclusion

A simplified intragranular description of dislocation density heterogeneities in the context of discontinuous dynamic recrystallization has been introduced in a full-field finite element level-set framework. This new formulation enables to account for the dislocation density heterogeneities especially near grain boundaries due to deformation

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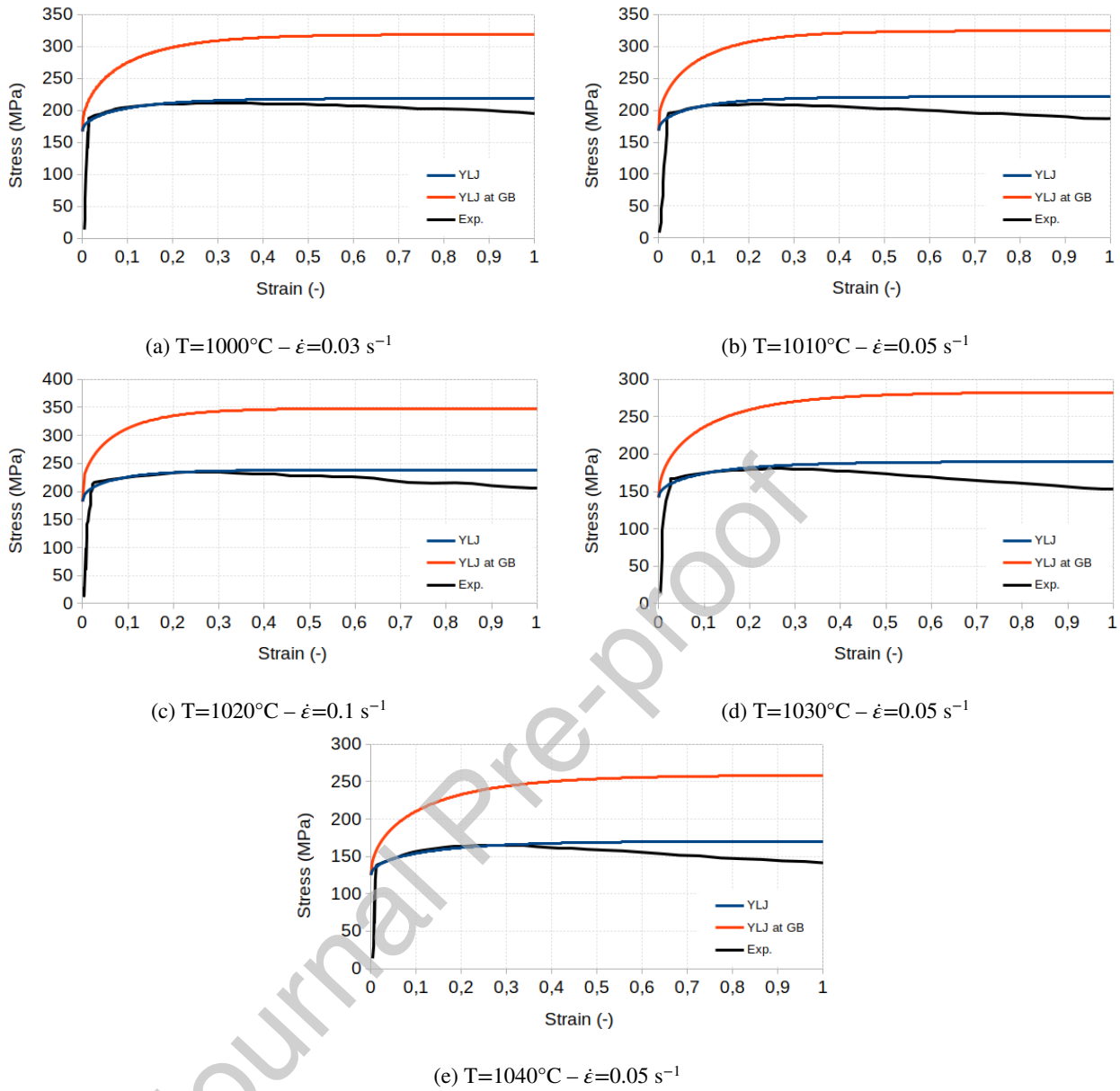


Figure 10: Predicted stress-strain curves versus experimental curves for dataset B.

incompatibilities between grains. The proposed model is quite straightforward and thus results in almost no additional computational time. The approach is rather pragmatic and may appear less attractive than for instance crystal plasticity but it remains based on experimental and physical observations and is drastically less demanding in terms of computational resources.

Recrystallized grain size and mean grain size predictions are improved for Inconel 718 superalloy and grain size distribution predictions appear to be also in good agreement with their experimental counterparts. Two distinct experimental datasets were used for model parameters identification and for validation. The material-dependent parameters identification procedure coupled with the model improvement enabled quantitative microstructure evolution predictions even in the case of a thermomechanical path comprising grain growth, dynamic and post-dynamic regimes.

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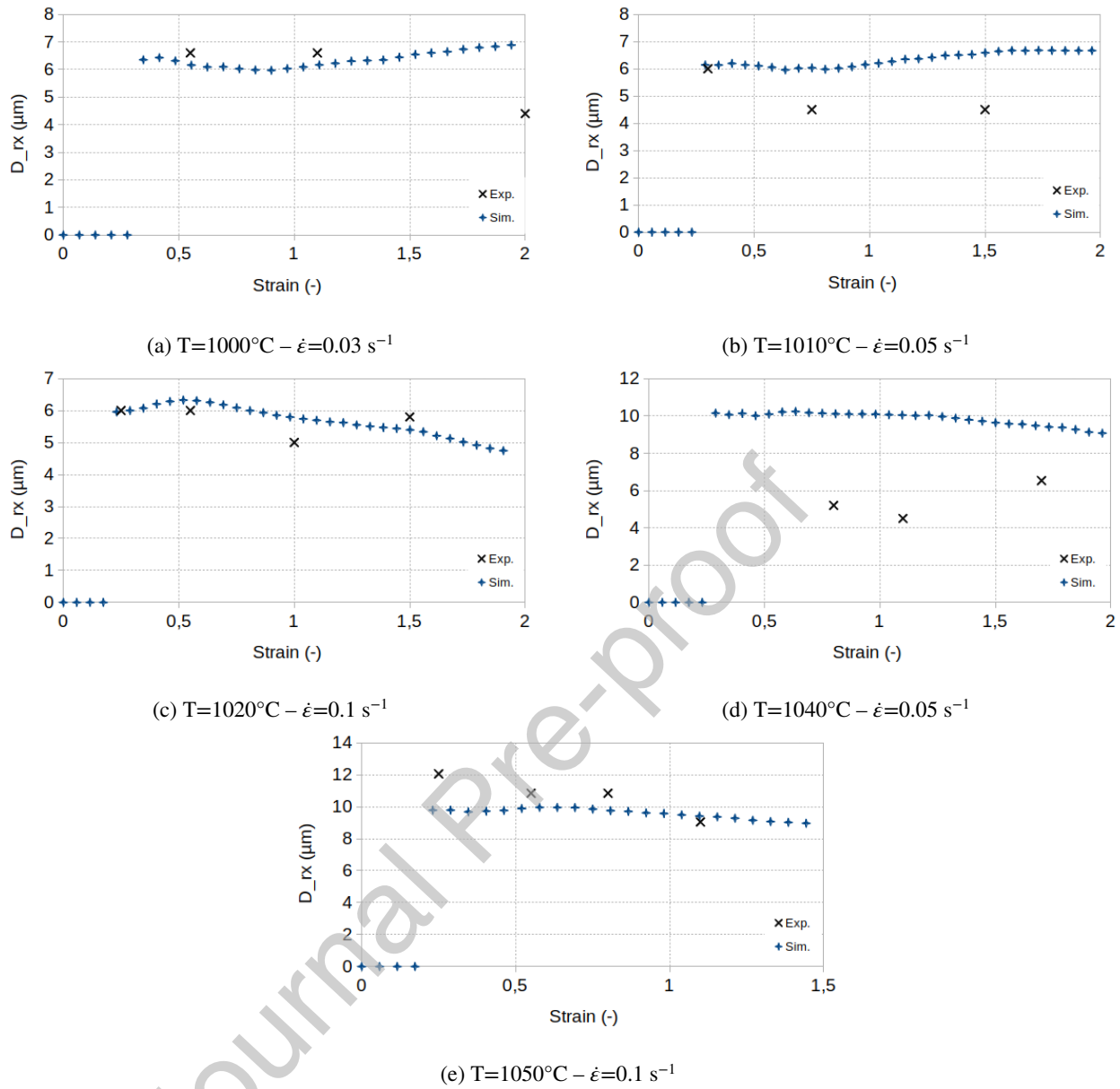


Figure 11: Recrystallized grain size with respect to strain level for dataset B.

To improve grain size distribution predictions, especially regarding discontinuous dynamic recrystallization and long post-dynamic holding time, several strategies are currently under study. A first study axis would be to account more accurately for dislocation density heterogeneities which may be done using crystal plasticity to describe dislocation density evolutions at the scale of the slip system [43]. This should enable a broadening of predicted RX grain size distributions during dynamic recrystallization. New developments have been recently published to account for grain boundary anisotropy either regarding grain boundary energy [15] and grain boundary mobility [33]. These developments are expected to improve the description of grain boundary heterogeneities which should in turn enables to better predict grain size distributions both during deformation (DRX) and during post-dynamic conditions.

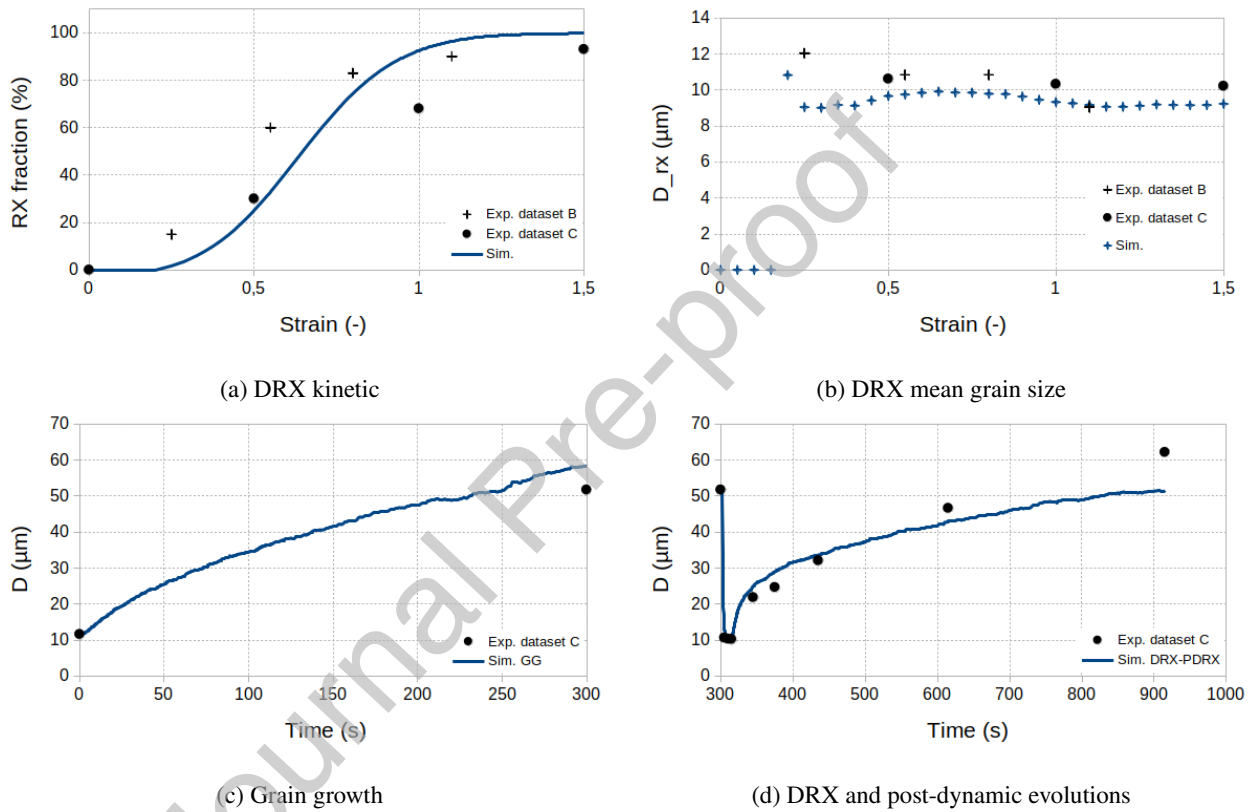


Figure 12: Simulations results for dataset C. (a) Recrystallized fraction and (b) recrystallized mean grain size evolutions in terms of strain level. For reference, experimental points from dataset B have also been plotted. (c-d) Mean grain size evolution with respect to time, (c) during GG and (d) during DRX and post-dynamic evolutions.

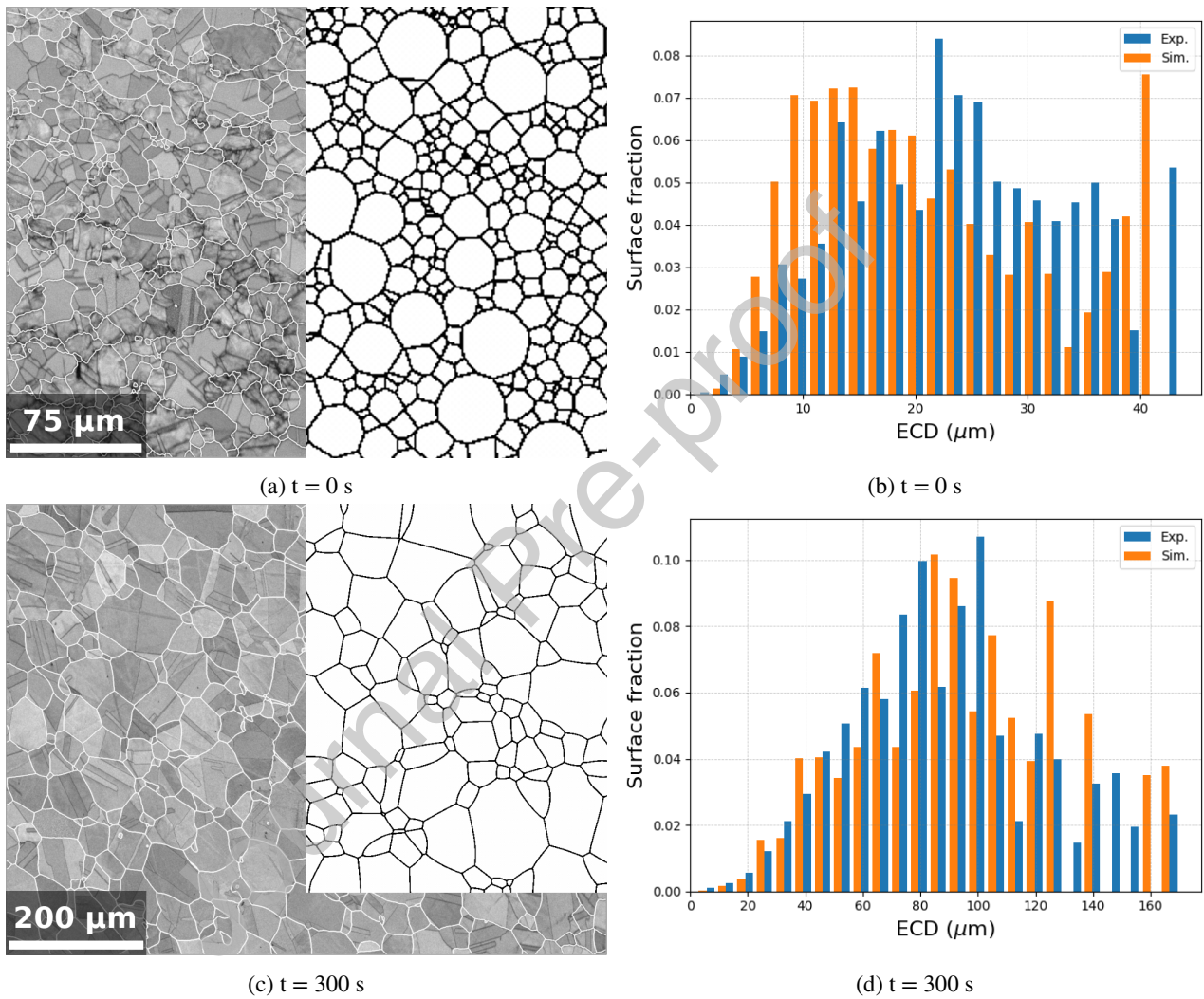


Figure 13: Grain growth simulation results for dataset C. Comparison of (a,c) predicted microstructures with experimental band contrast EBSD maps and (b,d) grain size distributions.

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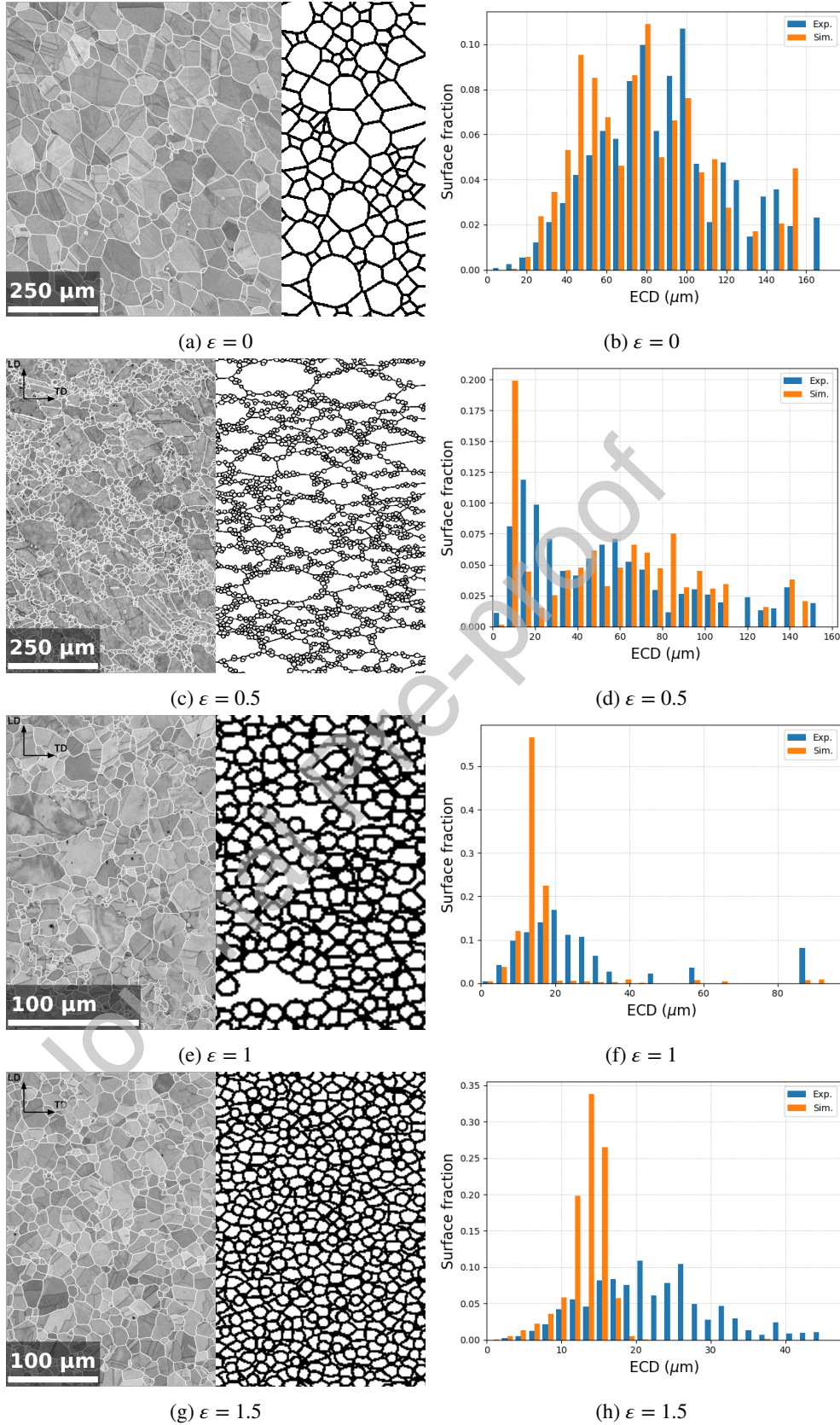


Figure 14: Discontinuous dynamic recrystallization simulation results for dataset C. Comparison of (a,c,e,g) predicted microstructures with experimental band contrast EBSD maps and (b,d,f,h) grain size distributions.

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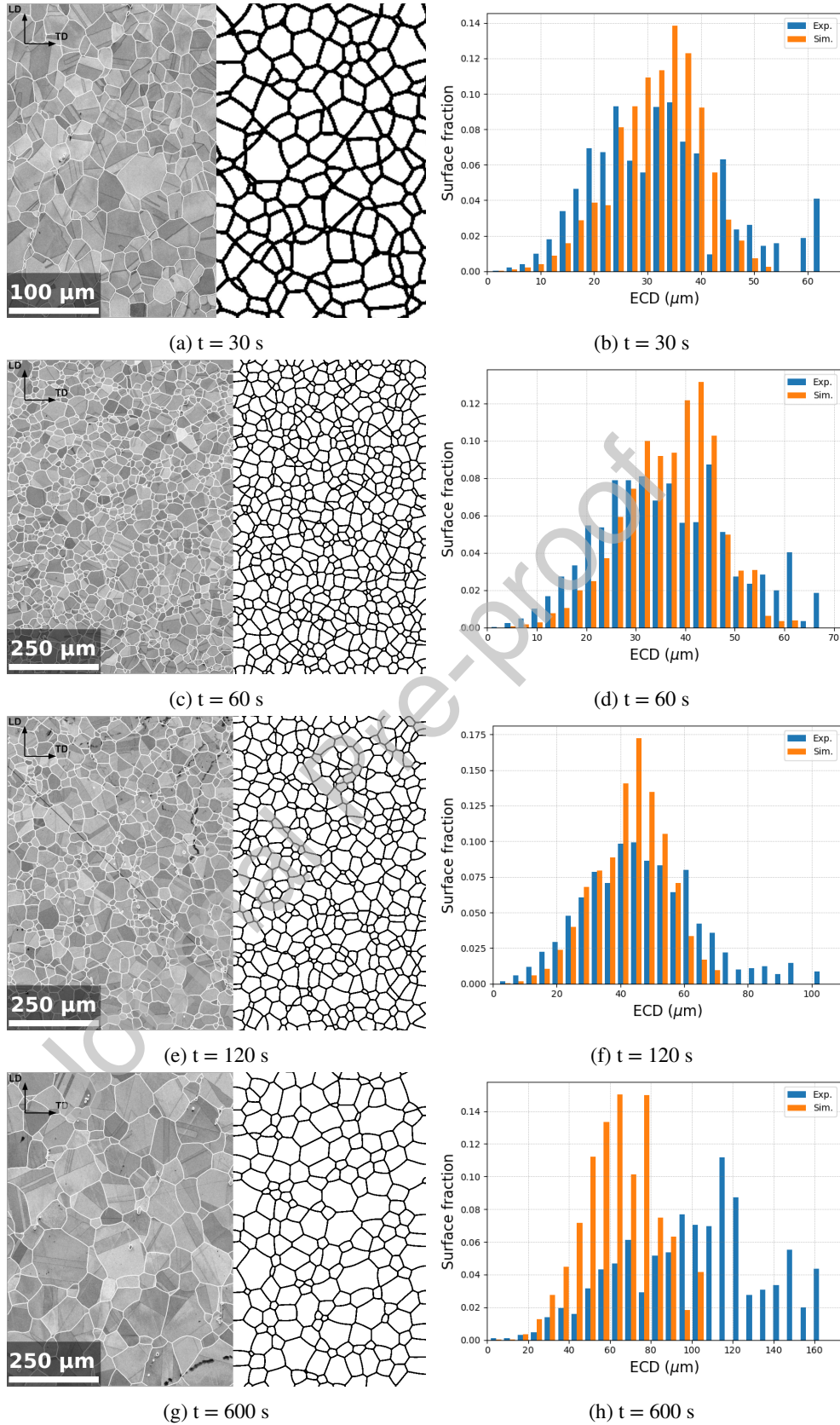


Figure 15: Post-dynamic simulation results for dataset C. Comparison of (a,c,e,g) predicted microstructures with experimental band contrast EBSD maps and (b,d,f,h) grain size distributions.

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Appendix

A. DRX material-dependent model parameters identification

Hardening and recovery (HR) parameters are identified first using an inverse analysis procedure consisting in minimizing the error between the Yoshie-Laasraoui-Jonas (YLJ) model and the experimental points (coming from a stress-strain curve) in order to obtain K_1 and K_2 values (resp. K_1'' and K_2'' for the local intragranular model presented in section 4.3.1). The Jonas method [22] is applied at first to obtain approximated values of the hardening/recovery material parameters, then parameters are refined by inverse analysis.

Regarding recrystallization kinetic, K_g and δ parameters are refined using direct inverse analysis with full field simulations.

A.1. Required experimental data

Ideally, dynamic recrystallization material parameters should be identified with a complete matrix of 27 mechanical tests (at least 3 temperatures (T) with 3 different strain rates (SR) for each temperature and 3 different strain levels to estimate RX kinetic). For each temperature, an other specimen for the initial state has to be analyzed. This leads to a total of 30 specimens in order to obtain a first set of identified parameters. The reproducibility of the obtained results will be automatically performed since at least 3 samples per thermomechanical conditions (T and SR) are necessary for the 3 strain levels.

Investigated temperatures and strain rates have to be kept closed enough from each other (a maximum of 50K and a variation of one order of magnitude for the strain rate between two mechanical tests should be considered) in order to limit errors during the multi-linear interpolation used in DIGIMU[®] software (v4.6) to access material parameters over the considered range of temperatures/strain rates. For the initial specimens, microstructure should be analyzed in order to obtain the grain size distribution ($\Sigma 3$ twin boundaries being filtered so that they are not taken into account for grain size measurements).

Figure 16 provides a scheme of a typical mechanical test used for DRX material parameters identification.

Different controlled and normalized mechanical tests can be considered in order to obtain σ - ϵ curves necessary to HR material parameters identification. Hot compression or torsion tests are usually used to investigate recrystallization kinetics. Compression tests enable to reproduce, in a more controlled way, industrial processes or at least some steps of complex forming/forging processes but may be limited if high strain levels have to be reached. In the latter, torsion tests may be used but with a possible effect of the deformation mode on *e.g.* RX kinetic.

Regarding interrupted tests used to estimate microstructural evolutions occurring during dynamic recrystallisation, different microscopy techniques may be adopted. Optical microscopy associated with a specific etching of GB may be sufficient to estimate evolutions of both RX fraction and RX grain size. This characterization method is particularly suited if a strong grain size contrast exists between initial grains and RX ones. If this is not the case, the use of a Scanning Electron Microscope (SEM) with an Electron BackScattered Diffraction (EBSD) detector can usually enable a precise estimation of RX fraction and grain size as well as overall grain size distribution evolutions. As detailed in Nicolaÿ *et al.* [34] RX and Non RX (NRX) grains can be discriminated using misorientation criteria such as Grain Average Kernel Average Misorientation (GAKAM or GAM) or Grain Orientation Spread (GOS). The latter may be coupled with a grain size threshold in order to filter more accurately RX grains from NRX ones.

In the case of a more restricted domain, other strategies can be employed in order to limit the number of samples in the design of experiments matrix. The strategy proposed in this work, detailed in the section 4.2.2 associated with Inconel 718 data coming from Zouari *et al.* [51] work, is based on the variation of the Zener-Hollomon (temperature compensated strain rate) parameter, denoted Z . Thermomechanical conditions (T, SR) are converted in their associated Z parameter and only a few conditions are used for identification following an increasing Z .

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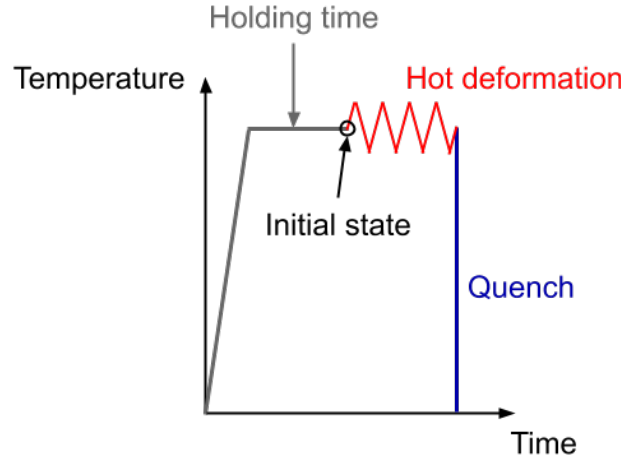


Figure 16: Scheme of a typical mechanical test used for hardening/recovery material parameters identification.

A.2. Identification of hardening and recovery parameters

In the following, a guided identification procedure is presented. To limit user dependency on the identification results, an interactive and graphical program has been developed (coded in python). A flow-chart of the program steps is provided in figure 17. Each step will be detailed in the upcoming subsections.

A.2.1. Homogeneous average dislocation density per grain

The Jonas' method [22] is used to process stress-strain curves in order to obtain a first estimation of the actual K_1 and K_2 value for each couple of test conditions (temperature and strain rate).

For each curve, the yield stress is identified graphically as the stress at 0.2% of plastic deformation. This initial value will then be refined during the inverse analysis step.

Only the first part of the plastic domain is considered for the identification of strain hardening and recovery. The elastic part of the curve as well as the plastic domain after $0.9 \times \epsilon(\sigma_{peak})$ (with σ_{peak} being the stress value at the peak stress (*i.e.* before softening)) are removed. A smoothing procedure is then used to limit the effect of experimental noise on the identification procedure:

1. Raw data are sampled to limit the number of points.
2. If necessary, a high-order polynomial is then used to smooth the experimental curve.

The next step of the identification relies on a graphical method used to obtain K_2 and to then deduce K_1 .

The Taylor's equation links the true stress σ to the mean dislocation density $\langle \rho \rangle$ in the case of an uniaxial loading:

$$\sigma = \sigma_0 + M_T \alpha \mu b \sqrt{\langle \rho \rangle}, \quad (28)$$

with σ_0 being the yield stress of the material, M_T the Taylor coefficient (≈ 3 in the case of a FCC material), α a material-dependent parameter associated with the formation of deformation substructures, μ the shear modulus and b the Burgers vector.

In the YLJ model, the dependence of the dislocation density on plastic strain is given by:

$$\frac{\partial \langle \rho \rangle}{\partial \epsilon} = K_1 - K_2 \langle \rho \rangle. \quad (29)$$

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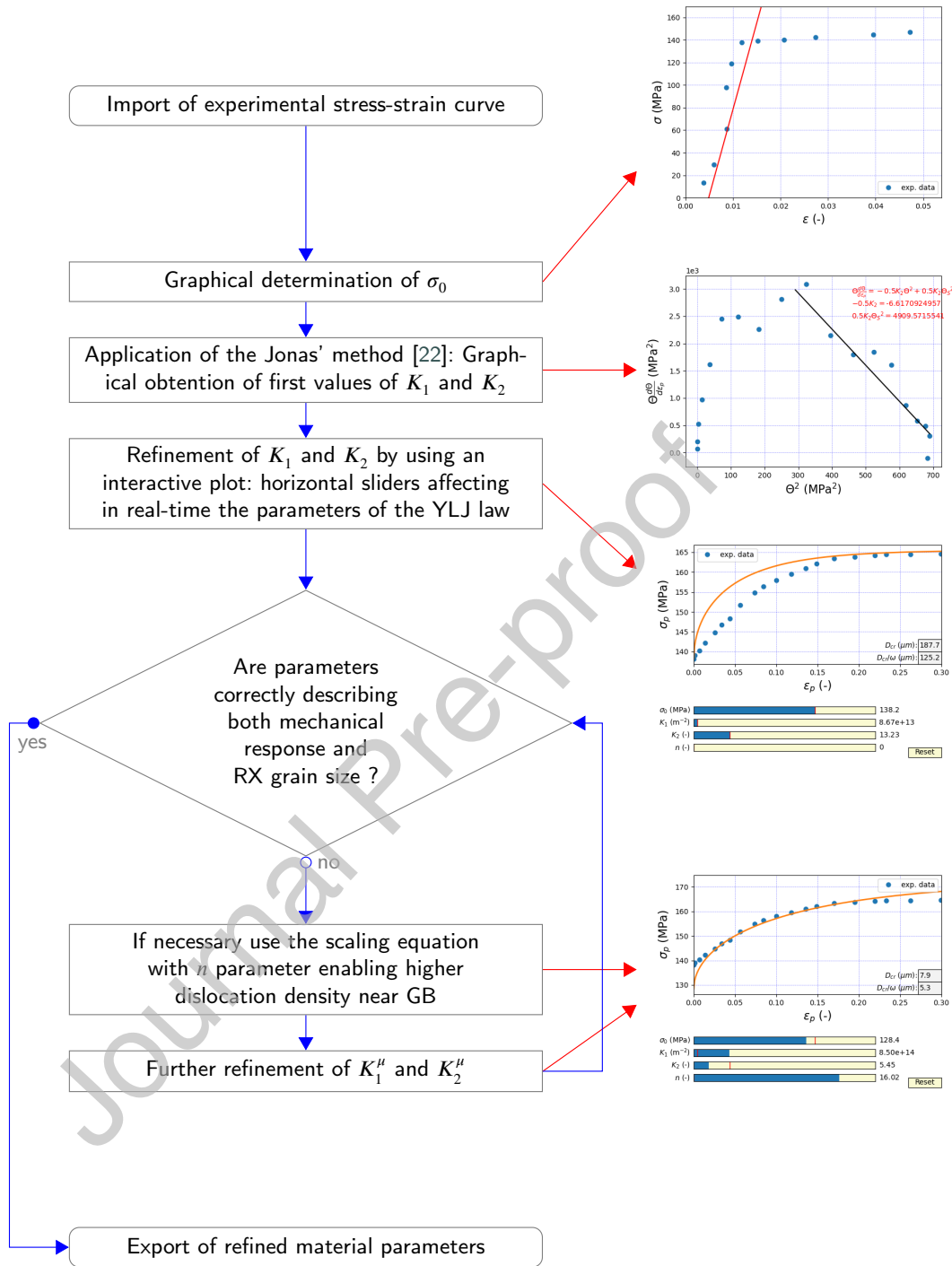


Figure 17: Flow-chart illustrating the main steps of the interactive and graphical program for hardening and recovery parameters identification. Plots are enlarged and details are given on each specific steps in sections A.2.1 and A.2.2.

Jonas *et al.* [22] demonstrated that if ϵ tends to infinity then the saturating stress can be expressed as:

$$\sigma_s = \sigma_0 + M_T \alpha \mu b \sqrt{\frac{K_1}{K_2}}. \quad (30)$$

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The saturating stress can be considered as the stress at which strain hardening and recovery, associated respectively to dislocations production and annihilation, are compensating each other.

In the following: $R = \sigma - \sigma_0$. Equations (28) and (29) are coupled, which results in:

$$\frac{\partial R}{\partial \epsilon} = \frac{M_T \alpha \mu b}{2\sqrt{\langle \rho \rangle}} (K_1 - K_2 \langle \rho \rangle). \quad (31)$$

Then by multiplying by R and using eq. (28):

$$\begin{aligned} R \frac{\partial R}{\partial \epsilon} &= \frac{(M_T \alpha \mu b)^2}{2} K_1 - \frac{(M_T \alpha \mu b)^2 \langle \rho \rangle}{2} K_2 \\ &= \frac{(M_T \alpha \mu b)^2}{2} K_1 - \frac{R^2}{2} K_2. \end{aligned} \quad (32)$$

And finally by introducing the saturating stress (eq. (30)) in the previous equation:

$$R \frac{\partial R}{\partial \epsilon} = 0.5 K_2 (\sigma_s - \sigma_0)^2 - 0.5 K_2 R^2. \quad (33)$$

The equation (33) is an affine function of $R \frac{\partial R}{\partial \epsilon}$ versus R^2 with a slope of $-0.5 K_2$ and an intercept given by $0.5 K_2 (\sigma_s - \sigma_0)^2$. By plotting those variables graphically it is possible to obtain K_2 and then σ_s . Eq. (30) is used to obtain K_1 :

$$K_1 = \left(\frac{\sigma_s - \sigma_0}{M_T \alpha \mu b} \right)^2 \times K_2. \quad (34)$$

Figure 18 illustrates the graphic determination of K_2 and σ_s used for the obtention of K_1 .

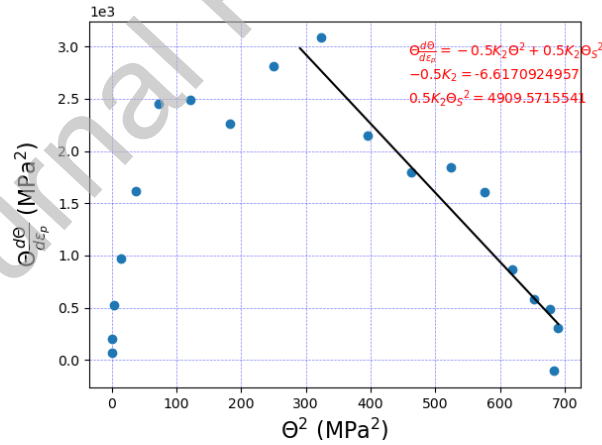


Figure 18: Graphic determination of K_2 and σ_s following the Jonas' method.

While figure 19 provides the smoothed experimental curve and the YLJ predicted curve with the K_1 and K_2 parameters obtained following the Jonas' method.

Once the initial parameters K_1 and K_2 have been obtained by the Jonas' method, it is possible to refine them by minimizing the error between the smoothed experimental curve and the predicted one.

To do so, YLJ model (eq. (29)) can be combined with the Taylor equation (eq. (28)):

$$\sigma = \sigma_0 + M_T \alpha \mu b \sqrt{\left(\rho_0 - \frac{K_1}{K_2} \right) \exp(-K_2 \epsilon) + \frac{K_1}{K_2}}. \quad (35)$$

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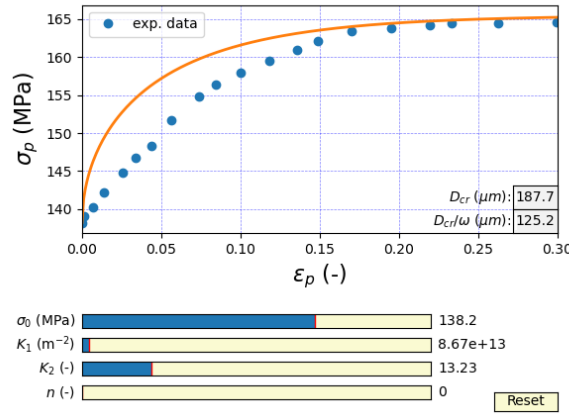


Figure 19: Experimental and sampled/smoothed stress-strain curves alongside with YLJ prediction after obtention of K_1 , K_2 by Jonas' method.

σ_0 is also modified during this step.

Figure 20 illustrates the predicted stress-strain curve obtained after K_1 and K_2 parameters refinement.

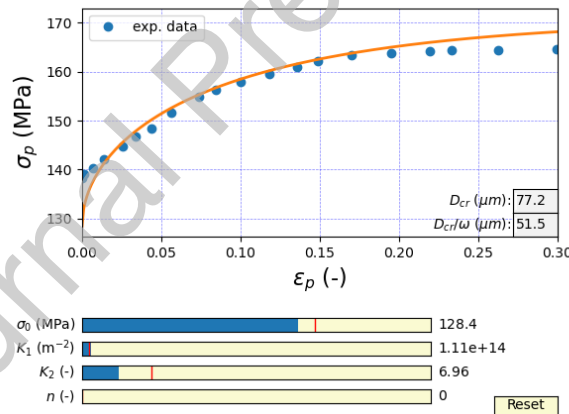


Figure 20: Experimental and sampled/smoothed stress-strain curves alongside with YLJ prediction after refinement of K_1 , K_2 .

The identification program allow the user to manually refine the material parameters but a more automatic inverse analysis with an optimization algorithm may be used.

As already stated in L. Maire PhD work [26], this two steps identification procedure enables to limit the interdependence between K_1 and K_2 . If only inverse analysis is performed, K_1 and K_2 might loose their physical meaning and compensate each other to fit experimental data. By using first the Jonas' method, the inverse analysis step starts on "physical" initial values. The main drawback of the actual procedure is the great dependence on the quality of the experimental curves used for the identification.

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A.2.2. Scaling equation and local estimation of dislocation density near grain boundary

In some materials, where intragranular dislocation density is highly heterogeneous, the assumption of considering only a mean value per grain may be limiting. It is especially detrimental regarding RX size predictions as already developed in section 4.2. The graphical and interactive program used for identification enables to vary in real-time the n parameter used in eq. (22) in order to progressively go from an homogeneous mean dislocation density value ($n = 0$) to a distribution of the dislocation density along the grain radius ($n > 0$). The latter is described by a power-law (cf. eq. (20) and (21)).

Figure 21 illustrates the results: no major modification in the mechanical response prediction (similar to the one in fig. 20). But a clear improvement of the RX grain size prediction: from about 75 μm to 8 μm . The latter being close to the experimental one for these thermomechanical conditions ($T=1040^\circ\text{C}$ and $\dot{\epsilon}=0.05 \text{ s}^{-1}$).

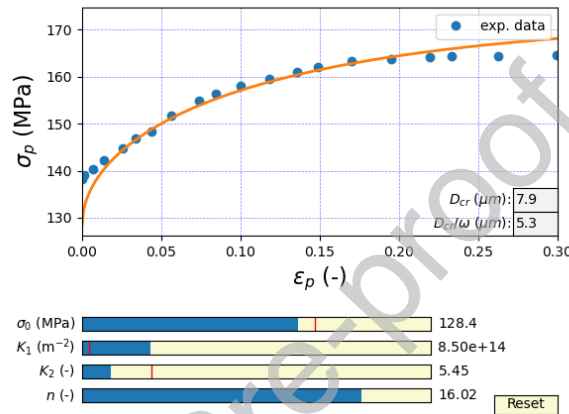


Figure 21: Experimental and sampled/smoothed stress-strain curves alongside with YLJ prediction after refinement of K_1^μ , K_2^μ using the n parameter.

A.2.3. Description of the evolution of K_1 and K_2 with mathematical equations

Finding the best mathematical functions to describe the evolution of K_1 and K_2 may be useful in order to have a continuous description of these parameters on the considered range of temperatures and strain rates.

There is no restriction regarding the mathematical functions to use. Jonas *et al.* [22] uses two linear relations respectively between K_1 and σ_p (peak stress value before softening) and between $\log(K_2)$ and σ_p . Maire [26] is using linear relations between K_1 and $\dot{\epsilon}$ and between K_2 and $\ln(Z)$ (Z being the Zener-Hollomon parameter).

The way to correctly describe the evolution of K_1 and K_2 regarding both temperature and strain rate is a complex question and work is still in progress to find the best compromise for the DIGIMU[®] framework.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

CRediT authorship contribution statement

B. Flipon: Conceptualization of this study, Methodology, Software, Data processing, Results analysis, Redaction. **N. Bozzolo:** Conceptualization of this study, Discussions, Corrections. **M. Bernacki:** Conceptualization of this study, Methodology, Discussions, Corrections.

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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