

Highlights

Robustness of Crystal Plasticity Parameters validation with Digital Image Correlation for fatigue modeling

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- The impact of different loading scenarios on the strain difference is evidenced.
- At low loads in fatigue regimes, the strain difference is below the noise. Calibrations on cyclic tests capturing cyclic behaviors are highly skewed by noise.
- Using a high load and with stress-control maximizes the signal-noise ratio of the strain difference.
- A necessary condition for a sound calibration with FEM-Updating is employed.
- It compares the measured DIC noise to the strain difference after a parameter variation.

Robustness of Crystal Plasticity Parameters validation with Digital Image Correlation for fatigue modeling

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Abstract

Advances in computational power has made microstructure-sensitive modeling more accessible in industry. For example, crystal plasticity models enable the understanding of the microstructure influence on fatigue crack initiation and propagation. However, these models require extended parameterizations with multiple coefficients, making it not only time consuming, but often inaccessible to engineers. Although multiple methods have approached parameters estimation by correlating models with macroscopic experimental measurements from a monotonic test, macroscale calibrations carry significant local uncertainties. In this sense, Digital Image Correlation (DIC) can offer mesoscale validation by providing a full-field measurement of strain that can be compared to the simulation. The main difficulty of this approach is the strain accuracy and the signal-to-noise ratio.

This work employs DIC to study parameter sensitivity and adequate parameterization strategies. We explore the strain difference after a model parameter variation using virtual experiments with different loading scenarios. A simple criterion comparing strain sensitivity to the model parameters and the measured DIC noise is proposed to assess the calibration robustness. Different case studies highlight the difficulty of validation under cyclic paths owing to a low signal-to-noise ratio. This is the main limitation for calibrations of models that aim to capture the cyclic behavior. We conclude with further recommendations to use DIC for model parameterization.

Keywords: Crystal-Plasticity Finite Element Method, Parameter calibration, Digital Image Correlation, Noise assessment, Signal-to-noise ratio, Lifting model

1. Introduction

1 A major challenge in the aeronautical industry is to reach sustainability over the next
2 decades, with the aim of net zero CO_2 emissions by 2050 [1]. A step towards this objective is
3 the development of new design for more efficient engines, which includes energy-efficiency and
4 an extended lifetime. Hence, we need accurate models to translate the mechanisms which
5 relate the fatigue life of engine components to their manufacturing attributes.

The evolution of fatigue damage has often been divided into distinctive stages, crack initiation, small, and long crack propagation [2]. Crack initiation is characterized by the local concentration of plastic strain that forms slip bands along the octahedral planes. For example, Fried et al. [3] observed that bands along with crack initiation occurred either in the grains with a high Schmid factor in grains with low misorientation. In the high cycle fatigue regime (low cyclic plastic strains significantly below the yield strength), crack initiation dominates fatigue life [4] and most of the lifetime is spent initiating cracks. Under these conditions, the mechanical behavior is highly dependent on several microstructural attributes such as the grain size, morphology, and orientation, which result in anisotropic plastic deformation.

Fatigue prognosis under low amplitude deformation requires microstructural-sensitive models, such as Crystal Plasticity (CP), to evaluate crack initiation driving force. CP models can represent heterogeneous plastic deformation at the grain level to inform Fatigue Indicator Parameters (FIPs) [5, 6], which serve as proxies of mesoscale crack initiation driving forces. These FIPs can be correlated to the number of cycles, and they often rely on the estimation of the plastic strain or energy consumed at the grain level. Hence, accuracy of life predictions is strongly correlated to the uncertainty in the CP predictions, which require robust calibration to match the material response.

Most commonly, model parameters are calibrated to macroscopic tensile tests. This approach often identifies parameters by minimizing the least squares error between the prediction and the experimental stress-strain curves [7, 8]. As explained by several authors [9, 10, 11], multiple sets of parameter values can result in similar macroscopic predictions, but may lead to different local responses at the grain scale [12]. As a result, the uncertainty of the constitutive model inputs at the mesoscale, propagates to the microstructure-sensitive life prognosis.

To mitigate these difficulties, inverse calibrations based upon full-field strain field data such as Finite Element Method Updating method (FEMU) (Fig. 1) have been proposed. This approach consists of an iterative method that makes the parameters vary. It compares the local difference between the model and the experimental strain fields at discrete locations of the sample measured with Digital Image Correlation (DIC). A least squares error or the Root Means Square of the residual between experiment and prediction is widely used as a cost function [13, 14]. It is minimized e.g. with bayesian or Hessian methods, to match the model with the measured strain values [15]. To calibrate CP parameters, Guery et al [16] used FEMU with a cost function weighted on both macroscopic and microscopic displacement. The experimental strain is obtained locally on the surface from a full-field by optical or scanning electron microscope (SEM) measurements.

The main challenge in such calibrations is the experimental noise that brings uncertainty to the identified parameters. SEM-DIC is commonly used with in-situ mechanical testing since it offers high magnifications and better resolutions. The method often involves procedures to reduce the noise from distortion during a scan [17], but at the cost of optimization steps. Jiang [18] successfully completed a CP-parameters validation by calculating experimental FIPs directly from SEM-DIC to obtain the location of the crack formation, yielding similar results to the numerical model predictions.

Cooreman et al. [19] and Lecompte et al. [20] pointed out that having enough heterogeneity in the strain field is paramount for a sound FEMU calibration. Pottier et al. [21] proved

this same observation by benchmarking inverse calibrations with several sample geometries with complex strain states and increasing strain field heterogeneities, after introducing a hole or with shear samples. They considered artificial noise and studied the consequent variation in the output parameters identification to measure their uncertainties. Further validation tests revealed a correlation between the level of heterogeneity and the accuracy of the predicted model despite the noise from DIC.

Inverse calibrations based on local features were largely performed with FEMU under monotonic loading, or in some cases under Ultra Low Cycle Fatigue regime with an applied macroscopic stress way above the yield strength [22]. This study explores FEMU calibrations with DIC under cyclic loading for a Nickel-based superalloy. We demonstrate the effects of low signal-to-noise ratio in LCF or HCF and analyze the ability of DIC to estimate CP parameters that control the strength. We further discuss the sensitivities and best configuration to minimize model inputs uncertainty. We conclude with a discussion of the potential and difficulties of the approach.

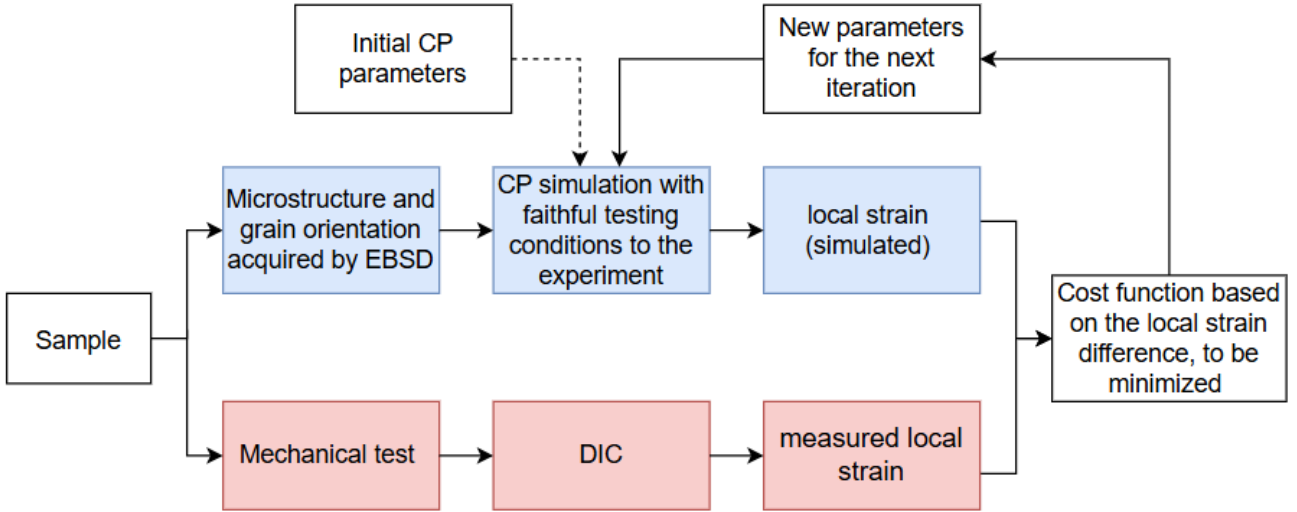


Fig. 1: Principle of the inverse calibration (FEMU)

2. Modeling Approach

2.1. Material

The study considers a cast Nickel-based superalloy MAR-M247 bar compacted by Hot Isostatic Pressing (HIP) to remove potential defects such as pores and solution heat-treated before annealing. This process results in a traditional Ni-based superalloy with a γ matrix and γ' precipitates and large grains with an average grain size of 1.56 mm measured by MTEX toolbox [23]. Fig. 2 presents the experimental response [24] for a single crystal oriented along the [001] direction, that was digitalized and fitted. This last step served to obtain the τ_c - γ curve required as input for the CP-model, for more details the reader can refer to Sayer et al. [25]. Table 1 summarizes the initial elastic [26] and plastic [27, 25] material parameters.

2.2. CP model

Our analysis assumes small strains, which is appropriate for low amplitude cyclic deformation. We decompose the total strain into two components; the elastic strain $\boldsymbol{\varepsilon}_e$ and the plastic strain $\boldsymbol{\varepsilon}_p$,

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p , \quad (1)$$

The Cauchy stress tensor is obtained from the generalized Hooke's law and expressed as a function of $\boldsymbol{\varepsilon}$, by combining Eq. 2 with Eq. 1. $\mathbb{C}$ refers to the anisotropic stiffness tensor, with the three components C_{11} , C_{12} and C_{44} of cubic materials,

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}_e = \mathbb{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p) , \quad (2)$$

The plastic strain rate is summed over the 12 slip systems plastic shear rate component $\dot{\gamma}^\alpha$ for an FCC material.

$$\dot{\boldsymbol{\varepsilon}}_p = \sum_{\alpha=1}^{n_{\text{slip}}=12} \dot{\gamma}^\alpha \mathbf{M}^\alpha , \quad (3)$$

where M^α is the Schmid factor, which multiplied by the tensile stress provides the resolved shear stress τ^α . The shear rate in Eq. 3 is linked to this resolved shear stress in the version of the flow rule by Cailletaud [28],

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{\tau_c^\alpha} \right|^m \text{sgn}(\tau^\alpha) , \quad (4)$$

τ_c^α is the critical resolved shear stress (CRSS) dictating if a plane is activated, and $\dot{\gamma}_0$ the reference shear rate. The exponent m is taken as $m \gg 1$ to minimize any viscoplastic behavior. Note that no latent hardening is considered for simplicity. The conjunct identification of these parameters brings computational complexity [16], which is not needed for the core aim here. Fig. 2 compares the initial calibrated model to the experimental tensile response.

Table 1: Material parameters at 25 °C. [26, 27, 25]

Type	Quantity	Value
Elastic	C_{11}	258.6 GPa
	C_{12}	167 GPa
	C_{44}	125 GPa
	$E_{[001]}$	127.5 GPa
Plastic	K'	1094 MPa
	n'	0.025
	$\dot{\gamma}_0$	0.001
	m	75

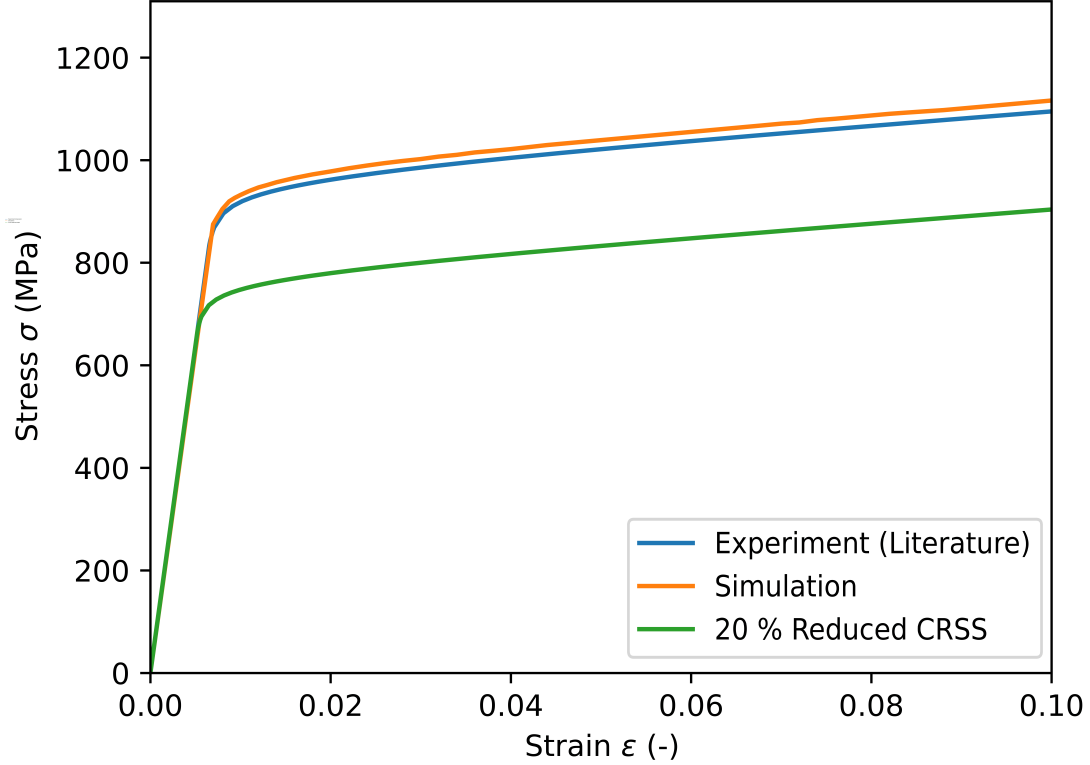


Fig. 2: Experimental fit [24] versus simulated macroscopic response of a single crystal loaded in [001] direction, and after a 20 % variation of the CRSS τ_c .

2.3. DIC noise

The DIC method relies on the conservation of the gray level. However, the image noise prevents a strict conservation so brings error to the measured strain, which propagates to the calibrated parameters. Hence, contrast quality and a good number of speckles are paramount to avoid noisy data, e.g. at least three speckle patterns per subset are advised in Ni-based superalloys [29]. An acid solution etched the γ' precipitates (speckles), before SEM acquisition. Moreover, a higher number of pixels per subset results in a noise reduction [30], but at the expense of spatial resolution [31]. We mitigate this effect with the high-resolution of SEM [17], that has a large field of view of 654 μm and a field distance of 15.01 mm. We measured the DIC noise from two images post-processed on Ncorr toolbox [32] using a strain radius of 5 pixels, a step size of 19 pixels and a high subset radius of 60 pixels. Thus, a medium to low noise level is expected (Fig. 12).

2.4. Strain sensitivity analysis after a model parameter variation

The use of DIC methods to validate CP parameters is possible as long as the strain measurements are sufficiently sensitive to stress changes. The approach is more accurate for materials with high hardening rate and becomes increasingly harder for materials that approximate a perfectly plastic response because a change in strain does not correspond to a change in stress. Thus, accurate parameter estimation requires lower DIC noise for shallower hardening. To study the required accuracy, we will examine synthetic strain fields from two

CP simulations with an artificial 20 % reduction of the CRSS, leading to lower strength (Fig. 2). A strain difference much larger than the noise means that DIC is effective to validate parameters and relatively insensitive to the noise. The flow chart in Fig. 3 summarizes the approach of the strain sensitivity ($\delta\epsilon_{xx}$) to a parameter variation.

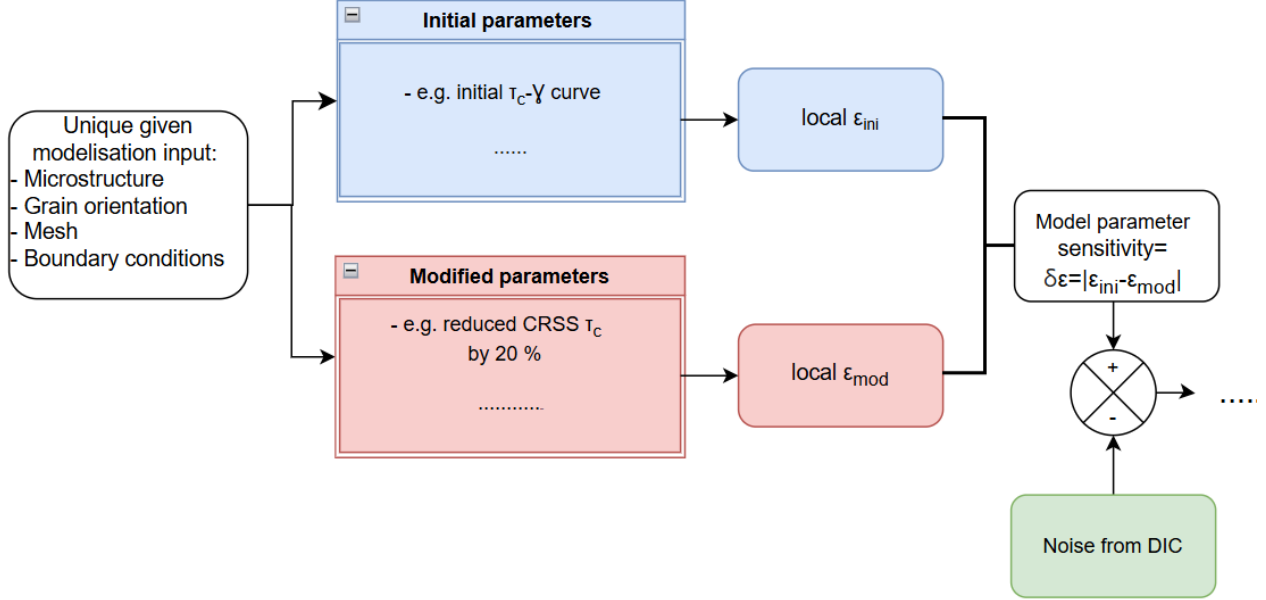


Fig. 3: Method for the parameter variation strain sensitivity study

2.5. Simulation, boundary conditions and mesh

The simulations employed two microstructures, one from Fried et al. [3] (Fig. 4a) and the other was scanned accordingly to part 2.3. They are named Microstructure A and B. One surface of the sample was acquired with EBSD and postprocessed with MTEX toolbox [23]. Since the sample thickness (1 mm) is lower than the average grain size, the sample is made of pseudo 3D-oligocrystals. Hence, the 2D-microstructure was extruded to form a 3D-part considering columnar grains and meshed with 15436 linear prism elements (Fig. 4b). The 3D mesh has only one element in the thickness direction. Heripre et al. [33] showed that increasing the number of elements although modifying the strain values had only negligible effects on the strain localization. We further consider the same mesh with an additional heterogeneity source, a new model was recreated with a circular hole, 0.5 mm in diameter, cut out from the mesh via GMSH [34] (Fig. 4c). As we focus on cyclic loadings, the assumption of a crack-free specimen in HCF enables to overlook discontinuities and consequently the crack tip mechanisms.

The analysis was further repeated for microstructure B in Fig. 5, which includes the effects of a stress concentration. The mesh contains 34796 linear triangular prisms and linear hexahedral elements assigned in GMSH [34] and the same boundary conditions as previously were applied (Fig. 5). The same strain sensitivity study that measures the strain difference after the parameter variation was followed, to quantify the influence of the sample heterogeneity.

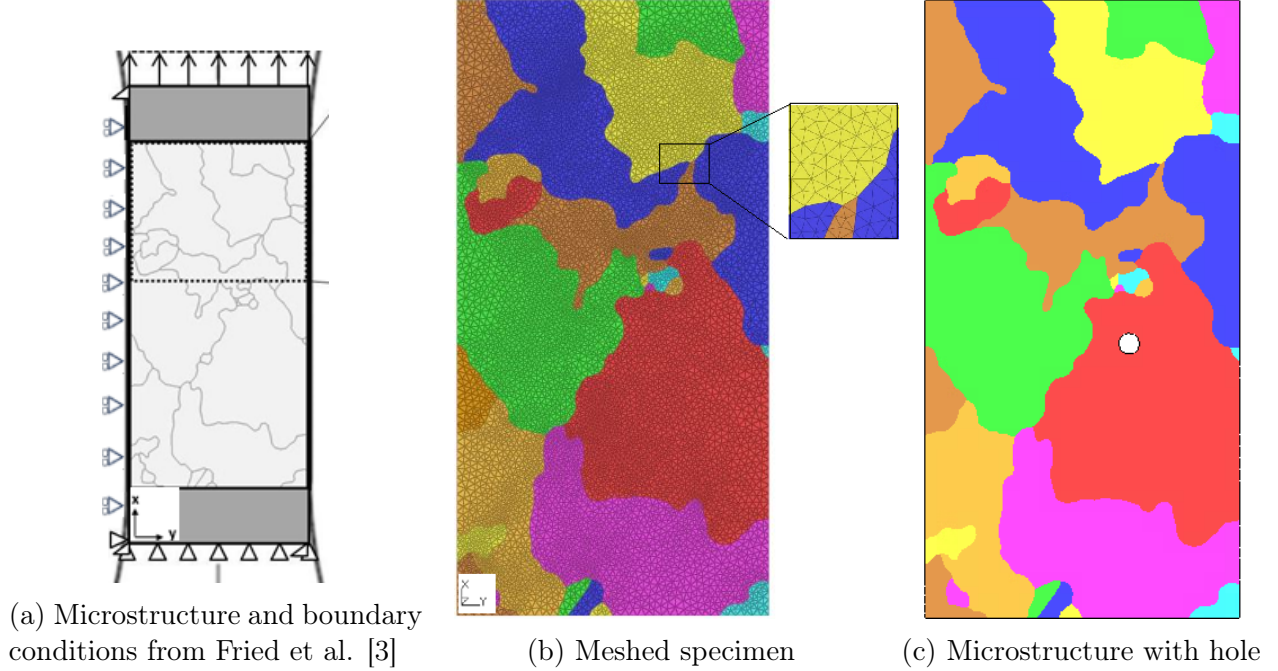


Fig. 4: Microstructure A used for the parameters sensitivity study (no significance of the color)

For all models, the boundary conditions constrained the displacement of the lower side and the displacement along the Y direction on the lateral side. At the upper side, the boundary conditions are homogeneous, so do not replicate a real experiment [35], which is not aimed, as we only simulate virtual experiments. We applied different stress or strain amplitudes using a triangular-shape ramp signal, to explore a loading impact on the strain difference. The local strain values were recorded at the tenth cycle and at the upper peak of the amplitude, and compared between both simulations with distinct CRSS values (Fig. 2).

3. Results

3.1. Influence of the load amplitude

First, we seek to evaluate the effects of reducing the CRSS on synthetic strain fields by computing the difference in absolute value between local strains in the original and the modified models, $\epsilon_{xx}^{\text{initial}}$ and $\epsilon_{xx}^{\text{mod.}}$. The strain difference ($\delta\epsilon_{xx}$) is calculated locally for each integration point, we then draw the distribution over all the integration points in Figs. 7a, 7b

$$\delta\epsilon_{xx} = |\epsilon_{xx}^{\text{initial}} - \epsilon_{xx}^{\text{mod.}}|$$

Fig. 6 (a) exemplifies the synthetic strain field difference computed for a monotonic load of 600 MPa using Microstructure A while Fig. 6 (b) presents the apparent Schmid factor M^α computed from the initial elements orientation and the load direction. Notably, the maxima of $\delta\epsilon_{xx}$ tend to lay close to the grain boundaries.

Figs. 7 a) and b) present the empirical probability density, as a function of $\delta\epsilon_{xx}$ from the strain fields obtained with CP simulations after 900 and 600 MPa applied loads. Figs. 7 c)

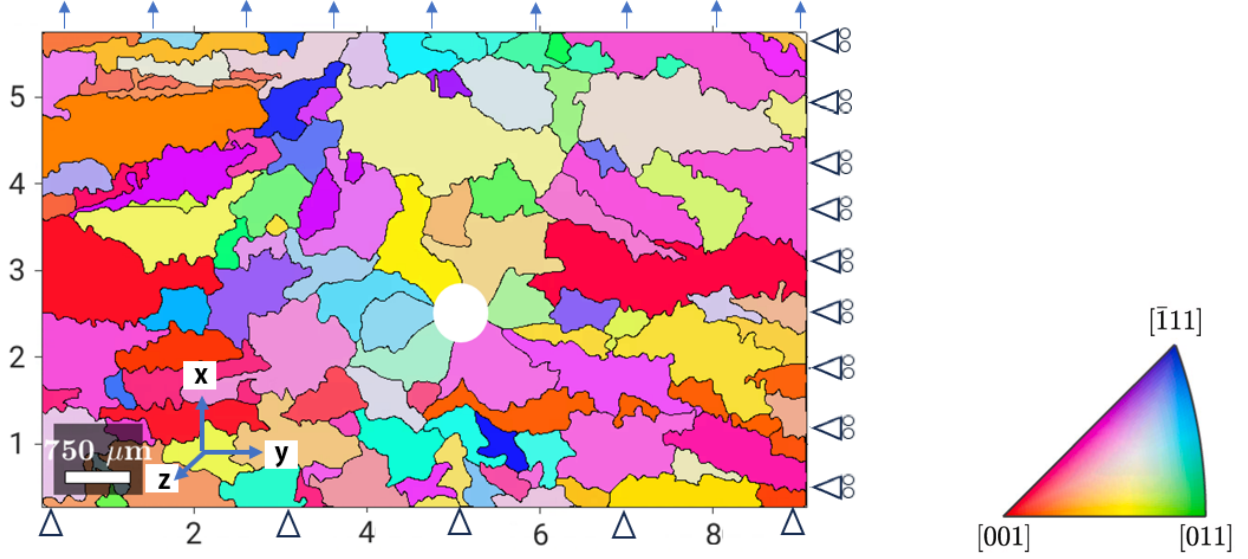


Fig. 5: Microstructure B; Inverse Pole Figure and boundary conditions, (colors from MTEX toolbox [23]; distances in mm)

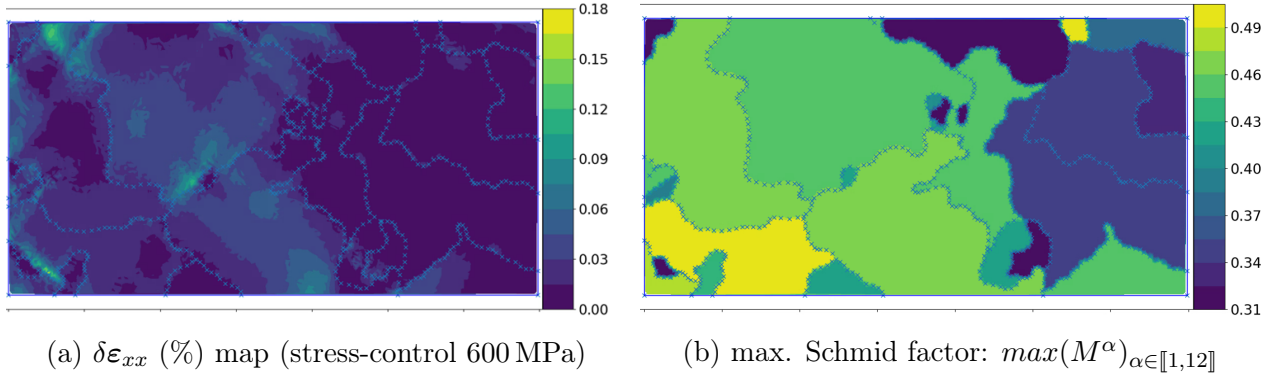


Fig. 6: $\delta\epsilon_{xx}$ field and maximum Schmid factor map (Microstructure A)

and d) further present $\delta\epsilon_{xx}$ versus the maximum apparent Schmid factor M^α . A maximum local strain difference of $\delta\epsilon_{xx} = 0.15\%$ (Fig. 7b) at 600 MPa compared to $\delta\epsilon_{xx} = 10\%$ at 900 MPa (Fig. 7a) suggests that some elements under the lower stress are still under elastic deformation. At the peak of the probability density, $\delta\epsilon_{xx}$ for 900 MPa (Fig. 7a), is significantly higher than under 600 MPa and also much higher than any typical noise values, so DIC is sensitive to a 20% CRSS variation. This effect favors the calibrations with tests under monotonic loadings over the LCF and HCF regimes, that employ lower loads.

Figs. 7d shows that the maxima of $\delta\epsilon_{xx}$ are for grains with highest Schmid factors $M^\alpha \simeq 0.475$ and then $M^\alpha \simeq 0.5$ (a horizontal line is a grain). This is expected, as grains with a high Schmid factor experience more plasticity [33]. Combined with the load effect on $\delta\epsilon_{xx}$, these grains should have higher strain differences. However, this is not always the case (e.g. $M^\alpha \simeq 0.45$), likely due to the influence of the specific neighbors. Also from Figs. 7c and 7d, there is no clear evolution of $\delta\epsilon_{xx}$'s scatter or median with M^α . A higher number of grains with uniform sizes is needed for more understanding on an orientation effect.

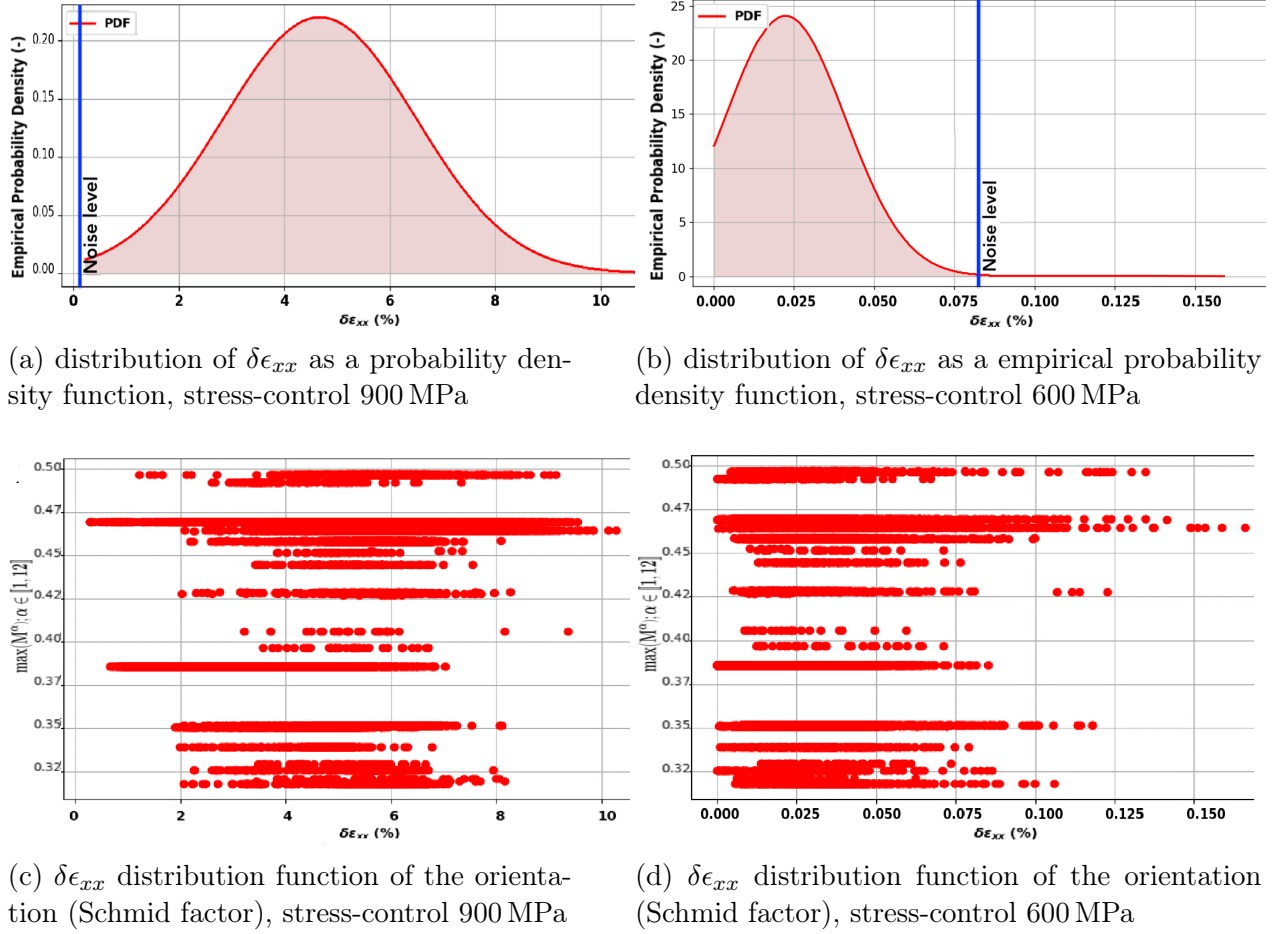


Fig. 7: Comparison of $\delta\epsilon_{xx}$ distributions computed from two synthetic strain fields under different loads for microstructure A

3.2. Strain versus stress-control

Under strain-control, the overall deformation is imposed, so both models must agree on the average strain. The comparison of the local strains can validate the crystal plasticity algorithms that partition the deformation increments into different slip systems. However, if enough plasticity is imposed, the elastic strains can be ignored and the slip partition is entirely a kinematic plastic response that becomes degenerated and independent of the stress. In other words, the imposed strain is partitioned almost without being affected by the stress. It means that there is no stress identification, and different stress forms are possible with the identified strain. This is a fundamental limitation that demonstrates that the stress-strain constitutive is not necessarily validated when measuring and controlling the imposed strains.

To evaluate these effects, we now deform the model under strain-control to compare the influence of the loading mode on the $\delta\epsilon_{xx}$ distribution for the original and modified response. Fig. 8 presents the stress-strain curve using an 0.15 mm imposed displacement on the original model. Here, the response reaches the same 900 MPa load amplitude applied in the stress-controlled simulation (subsection 3.1). Hence, compared to Fig. 7a, only the loading mode influence is highlighted as no amplitude effect from subsection 3.1 comes into play.

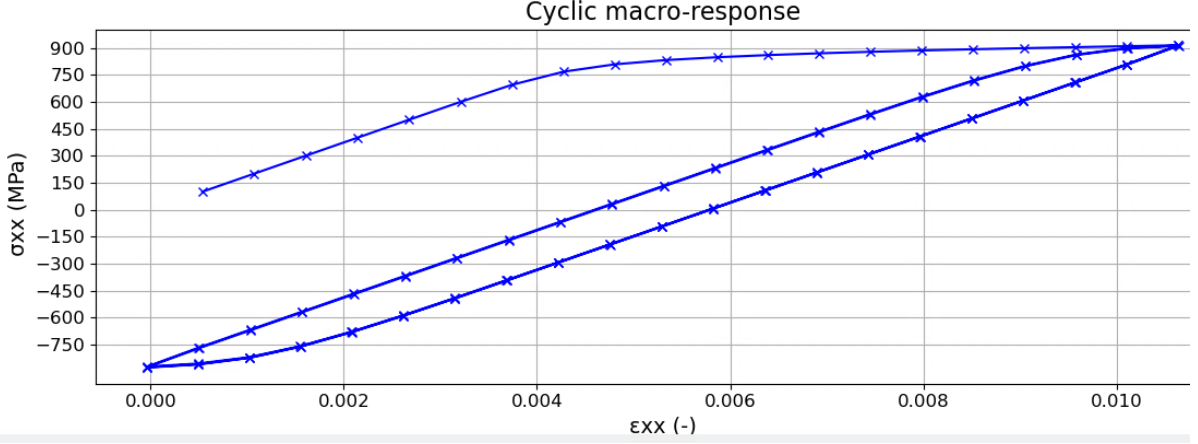


Fig. 8: Stress-strain curve strain-control disp.=0.15 mm, (equivalent load of 900 MPa as in Fig. 7a)

With strain-controlled simulations (Fig. 9b), at the peak of density the strain difference $\delta\epsilon_{xx} \simeq 0.04\%$ is much lower than the associated stress-control $\delta\epsilon_{xx} \simeq 4.5\%$ (Fig. 9a). Despite the high amplitude of 900 MPa, favorable to high values of $\delta\epsilon_{xx}$, the strain-control mode is less efficient to differentiate the strain fields from both CRSS values. This effect can be attributed to the strain-controlled mode, the macroscopic strain $\delta\epsilon_{xx}^{\text{macro}}$ is imposed for both simulations, $\delta\epsilon_{xx}^{\text{macro}} = 0$. As a result, a constraint that links the local differences $\delta\epsilon_{xx}^{(k)}$ together, does not enable to reach high values as formalized in Eq. 5.

$$\delta\epsilon_{xx}^{\text{macro}} = \sum_{k=1}^{N_{\text{int.point}}} \frac{\delta\epsilon_{xx}^{(k)}}{N_{\text{int.point}}} = 0 \quad (5)$$

In contrast, with stress-control, two distinct values of the CRSS lead to significant macroscopic strain variations $\delta\epsilon_{xx}^{\text{macro}}$ (Fig. 2), implying necessarily high local $\delta\epsilon_{xx}^{(k)}$ values. However, the joint identification of several model parameters is inherently non-deterministic, meaning that different parameter sets can produce similar macroscopic responses [12], i.e. $\delta\epsilon_{xx}^{\text{macro}} \simeq 0$ even with stress-control.

3.3. Influence of a hole on $\delta\epsilon_{xx}$

Fig. 11 shows the $\delta\epsilon_{xx}$ distribution for Microstructure A with a hole. Compared to Fig. 11a, the same simulation (600 MPa), but without a hole, the maximum of $\delta\epsilon_{xx}$ was increased four times (Fig. 11b). Fig. 10 presents the strain difference field. The maxima are concentrated in the vicinity of the hole, which is further confirmed by Fig. 11c, the selection of the Region of Interest (ROI) around the hole shifted the peak to the higher sensitivity domain, meaning a lower proportion of elements, which are corrupted by noise. Interestingly in Fig 10, an influence is also in other grains far from the hole (e.g. grains 8 and 9, label in Fig. A.19). Hence, a stress concentration increases the local strain difference, which reduces the error on the calibration.

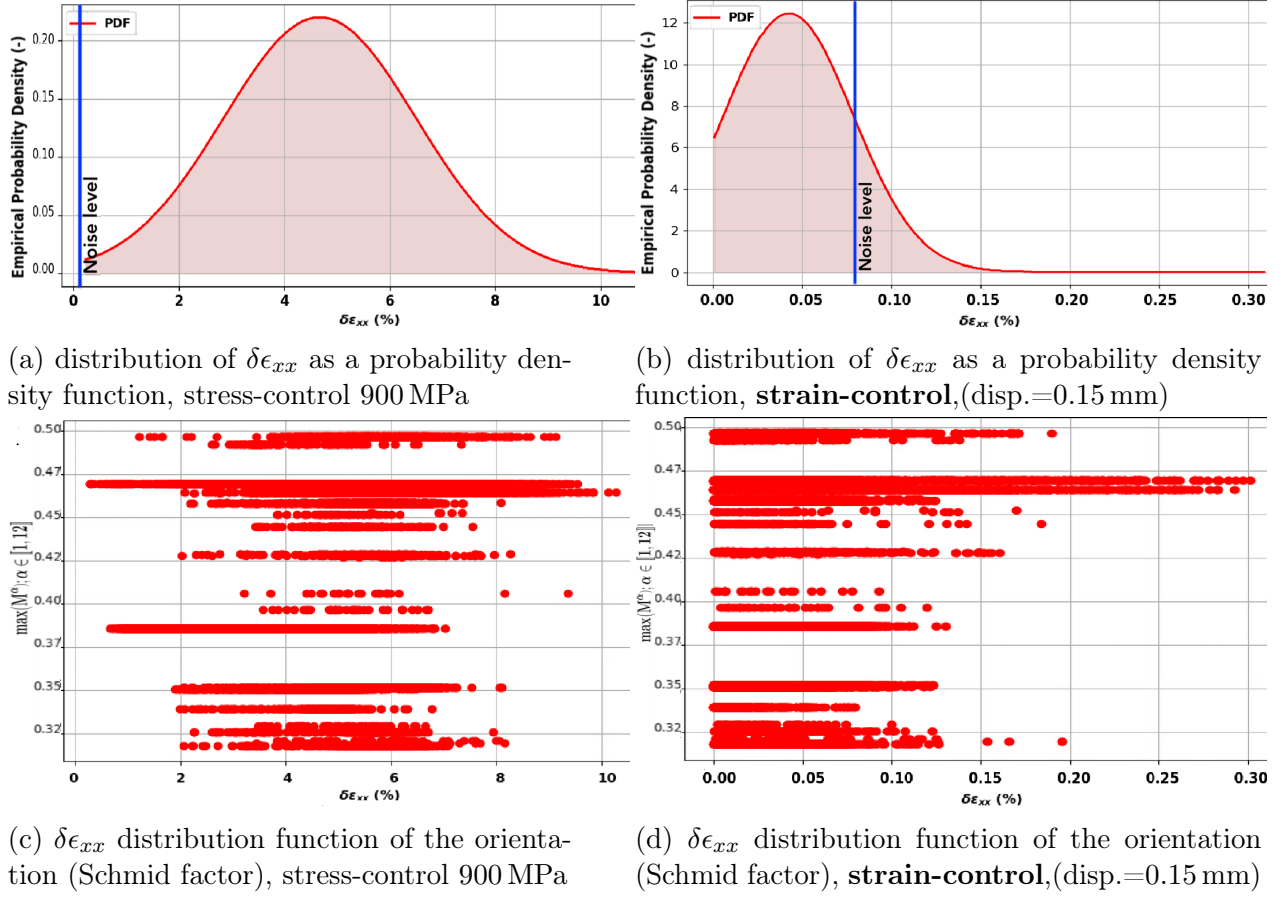


Fig. 9: Sensitivity comparison between stress- and strain-controlled simulations under a similar load of 900 MPa, (Microstructure A)

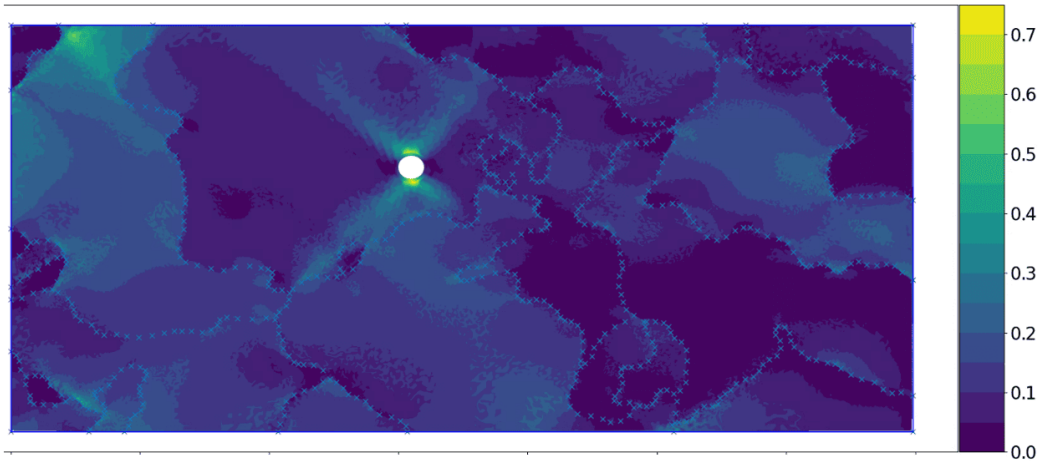


Fig. 10: $\delta\epsilon_{xx}$ (%) map with a hole in the center (map to compare with Fig. 6a), 600 MPa

3.4. DIC uncertainty and criterion on the strain difference

To quantify the DIC uncertainty, two images are taken; a reference one and the other after a sample repositioning, without any load application. The strain difference provides

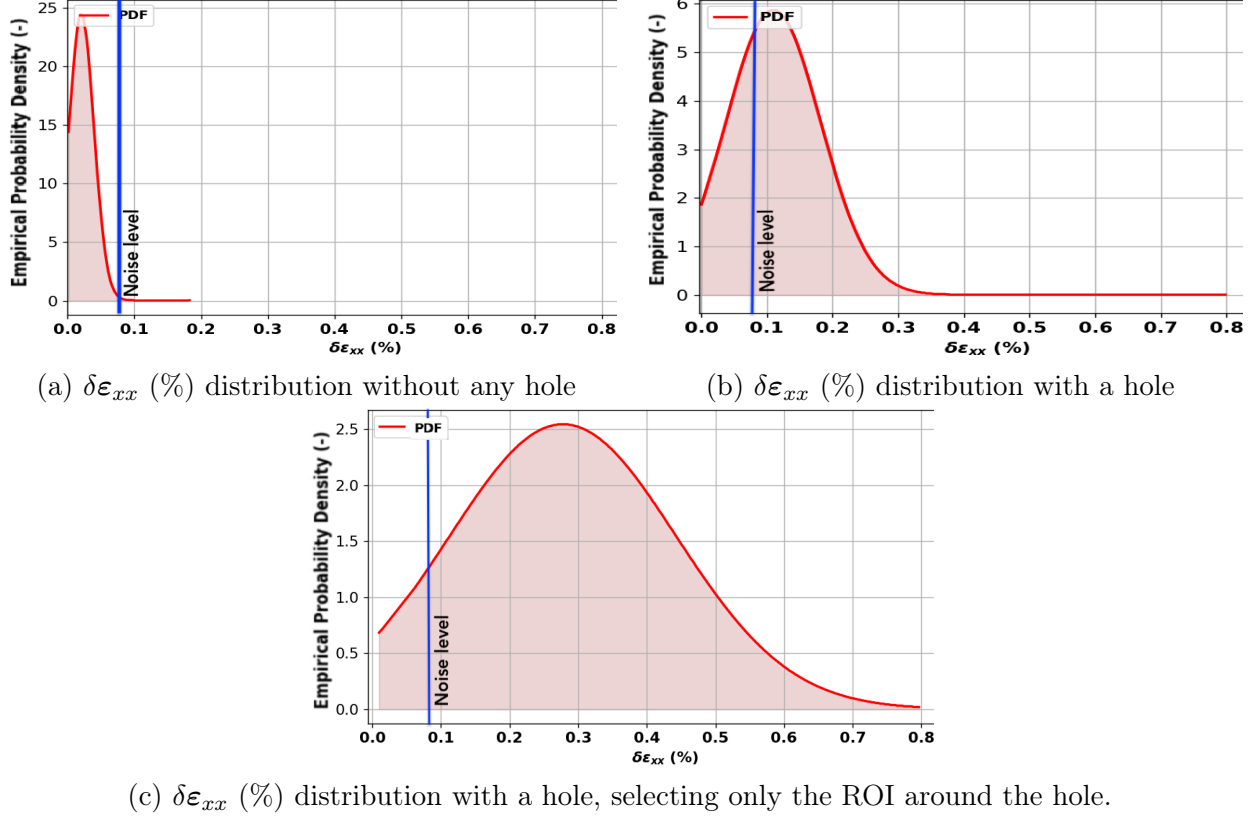


Fig. 11: Influence of a hole on the distribution of $\delta\epsilon_{xx}$, stress-control with 600 MPa

the noise (Fig. 12a). Although the noise can get worse under dynamic conditions, when the speckles are deformed and the tracking is more compromise, the present method is most commonly employed even in fatigue analysis [31]. It often follows a Gaussian distribution, Fig.12b shows the fit with a good coefficient of determination of 0.99. Its standard deviation $\sigma_{\epsilon;\text{DIC}}$ is often taken to assess the level of strain uncertainty with DIC [36, 37]. Typical noise levels with SEM-DIC are around $\sigma_{\epsilon;\text{DIC}} = 0.1\%$; e.g. Guery et al. [37], reported noise values between 0.09% and 0.15%. Fig. 12b shows the experimental distribution with the standard deviation $\sigma_{\epsilon;\text{DIC}} = 0.08\%$.

For DIC methods to resolve strain differences, they should have a strain noise $\sigma_{\epsilon;\text{DIC}}$ at least lower than $\delta\epsilon_{xx}$ statistically described at the peak of density (Eq.6). This is a necessary criterion, but implies a poor signal-to-noise ratio so is not sufficient.

$$\delta\epsilon_{xx} > \sigma_{\epsilon;\text{DIC}} \quad (6)$$

Eq. 6 is satisfied for the previous results when the applied load is high (900 MPa) (Fig. 7a), but most elements do not fulfill Eq. 6 at a low load typical of fatigue conditions, (600 MPa) (Fig. 7b) so that a CRSS parameter could not be validated accurately under these testing conditions. The same observation is made even higher loads but using strain-control as previously explained.

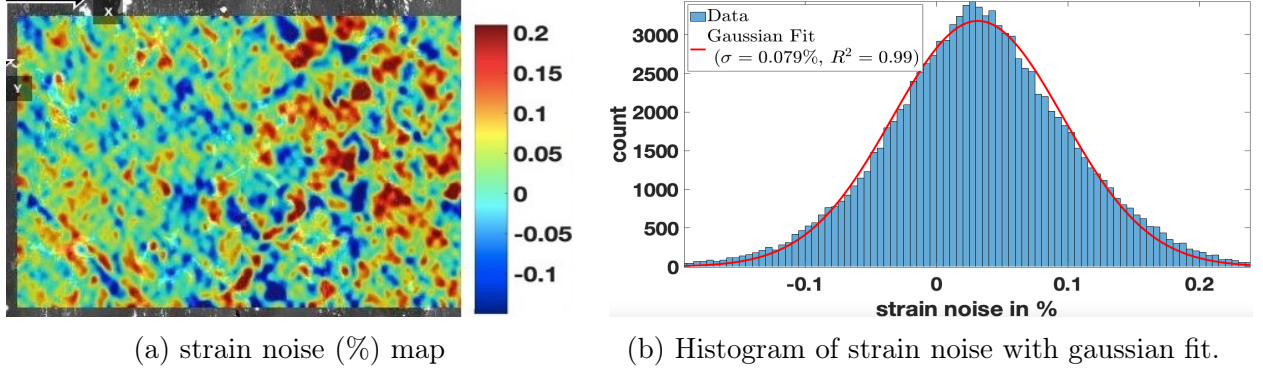


Fig. 12: Noise assessment, strain difference of two stationary images after sample repositioning

3.5. Effects of slip heterogeneity

One of the most difficult validation aspects of CP is the local response, which has lead to a lack of realistic heterogeneity among grains [38]. Hence, we can increase grain-to-grain heterogeneity in the model without affecting the macroscopic response by making $\dot{\gamma}_0$ a function of the grain orientation. $\dot{\gamma}_0$ is not constant but distinct to each grain, while ensuring that the average value among grains still equals the initial value.

The proposed distribution of $\dot{\gamma}_0$ in Table A.2, is such that $\dot{\gamma}_0$ is proportional to the Schmid factor (Eq. 7), this simplified trend meets the physical principles proposed in [38] and [39] demonstrated in Appendix A.1.

$$\dot{\gamma}_0 \propto \max(M^\alpha)_{\alpha \in [1,12]} \quad (7)$$

We performed a similar analysis to quantify $\delta\epsilon_{xx}$ between the strain computed with constant and the strain with the heterogeneous variable $\dot{\gamma}_0$. Since in both cases the average $\dot{\gamma}_0$ value remains the same, the macroscopic response is not affected as shown in Fig. 13. This demonstrates the almost perfect overlap of both macroscopic responses using constant or heterogeneous $\dot{\gamma}_0$.

Fig. 14a presents the map of the strain difference between the initial homogeneous constant $\dot{\gamma}_0$ and the heterogeneous variable. Compared to 6 (b), the DIC analysis could not identify significant differences for the high Schmid factor grains and is not sensitive to intragranular slip heterogeneity for those grains. Thus, DIC agreement between model and experiment does not fully validate the model form and the mechanisms controlling $\dot{\gamma}_0$.

The $\delta\epsilon_{xx}$ distribution under a load of 1000 MPa stress-control (Fig. 14b) and associated strain-control (Fig. 16) shows that at the density peak, the stain difference is higher than the measured noise $\sigma_{\epsilon, \text{DIC}}$. In contrast, under a lower load of 600 MPa below the yield strength (Fig. 15), even the maximal value 0.014 %, is negligible compared to the noise level.

The strain-control (Fig. 16) and corresponding stress-control (Fig. 14b), both presented a similar $\delta\epsilon_{xx}$ distribution. This result differs from the subsection 3.1, where after the CRSS variation, $\delta\epsilon_{xx}$ was locally significantly higher with the stress-control compared to strain-control. So this effect can not be generalized, and is attributed to the large macroscopic difference after the CRSS variation as explained in subsection 3.2, which was absent upon the $\dot{\gamma}_0$ variation (Fig 13).

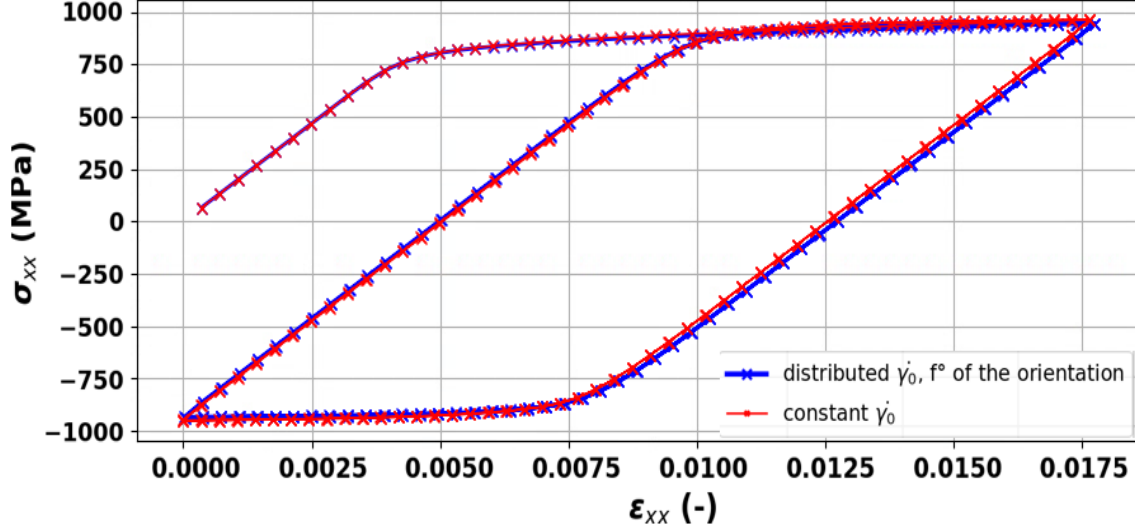
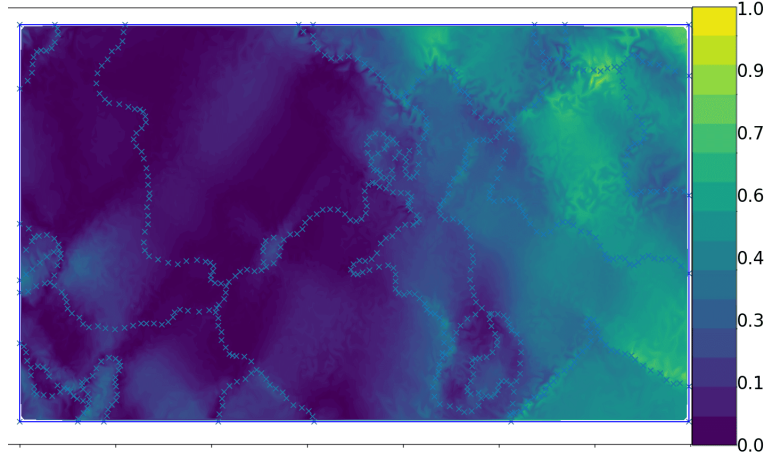


Fig. 13: Stress-strain curves from homogeneous (red) and heterogeneous (blue) $\dot{\gamma}_0$ (simulations strain-control)

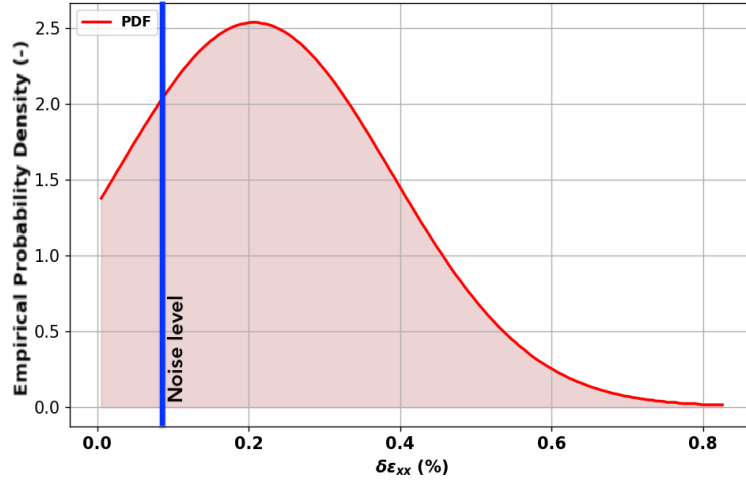
4. Discussion

The analysis highlighted that DIC can be used for validation when stresses or strains are high enough such that $\delta\epsilon_{xx}$ at the density peak is significantly above the noise level. This constitutes a severe limitation for small strain cyclic deformation and may prevent DIC from being effective in validating constitutive models. This principle aligns with other identifications from previous studies. Guery et al. [16] showed that the displacement difference after a variation of hardening parameters was higher than the DIC resolution in pixel only at the last steps of a tensile test when most local parts of the sample had plasticized. Other calibrations [35, 40], mentioned a high applied amplitude e.g. a strain reaching 14 % for Goulmy et al. [41], and reported a decreasing cost function, so the identification was not detrimentally affected by the noise. Consequently, DIC is more amenable to validate the response of materials under significant plastic deformation, and difficult for complex loadings in LCF or HCF as the low load depletes the signal-to-noise ratio.

To assess the reproducibility of the results from subsection 3.1, the same procedure with the 20 % CRSS reduction was repeated with Microstructure B. Fig. 17 presents the $\delta\epsilon_{xx}$ distribution. It differs from the distribution with the previous microstructure A (Figs. 11b and 11c), where the maximal value of $\delta\epsilon_{xx}$ is twice higher. This difference reveals that the previous quantitative results are microstructure-dependent, so the success of an identification can vary significantly between two microstructures. This idea was already suggested by Guery et al. [16]. Given the measured value of noise $\sigma_{\epsilon;DIC} = 0.08\%$, Fig 17a highlights the limitations of DIC since no integration point satisfies the necessary criterion Eq. 6. Thus, DIC could not distinguish between the two parameters values because of noise corruption and FEMU would result in an incorrect value of the CRSS. We note that the 20 % change in CRSS is an arbitrary choice to evidence the limitation of DIC and therefore only provides a lower boundary of the parameter uncertainty. Since the DIC can not distinguish the 20 % reduction from the initial parameter, it would not distinguish even smaller differences.



(a) $\delta\epsilon_{xx}$ (%) map



(b) distribution of $\delta\epsilon_{xx}$ (%), 1000 MPa

Fig. 14: Distribution of $\delta\epsilon_{xx}$ between homogeneous and heterogeneous $\dot{\gamma}_0$ (stress-control; 1000 MPa, microstructure A)

4.1. Prospect for calibration improvements

Our results presented two scenarios in which the macroscopic response is not affected but the local strains present significant differences. This corresponds to the main weaknesses of the macroscopic calibrations. Hochhalter et al. [12] have also pointed out that a calibration of several parameters on a stress-strain curve is not deterministic. As a result, the prediction of the mechanical responses based on grain-level information is not rigorously validated.

Owing to the poor strain-to-noise ratio in cyclic calibrations aimed at capturing the fatigue behavior, we propose a strategy to avoid noisy data. The approach introduces a weighting of the different Gauss points in the cost function, to give more relevance to the elements with high $\delta\epsilon_{xx}$ values such as around the hole (Fig 10). Weighting could also consider the local noise values from DIC, to discard the noisiest integration points as well [42]. Similarly, differential weighting to some parameters can be implemented for grains with

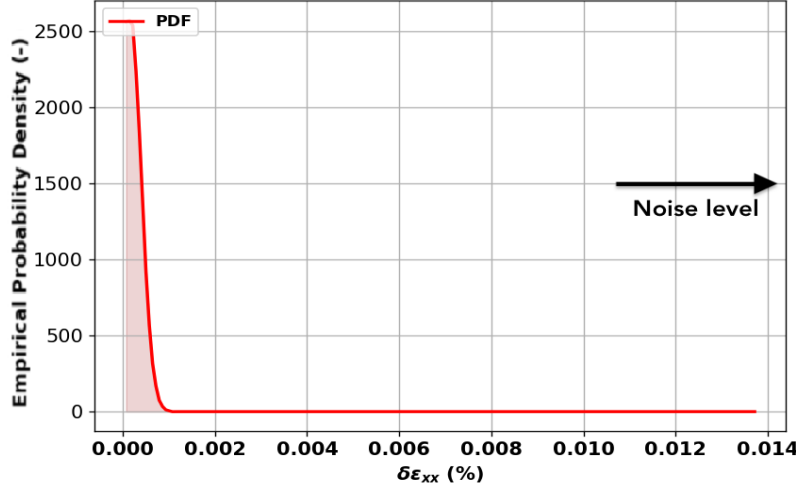


Fig. 15: Distribution of $\delta\epsilon_{xx}$ (%), stress-control 600 MPa for homogeneous and heterogeneous $\dot{\gamma}_0$

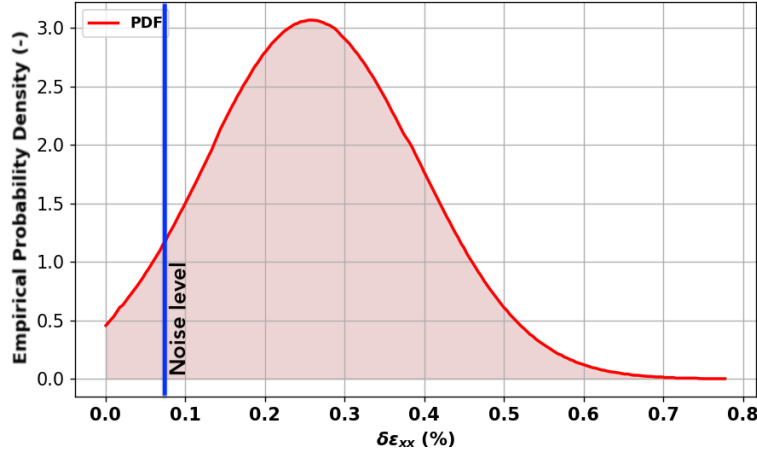
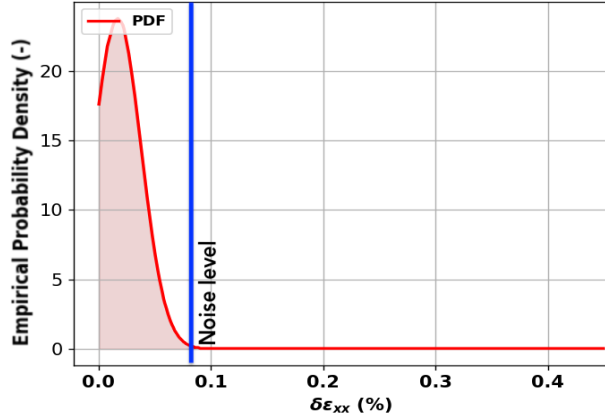


Fig. 16: Distribution of $\delta\epsilon_{xx}$ (%), strain-control, equivalent max. load of 1000 MPa for homogeneous and heterogeneous $\dot{\gamma}_0$, to compare with Fig. 14b

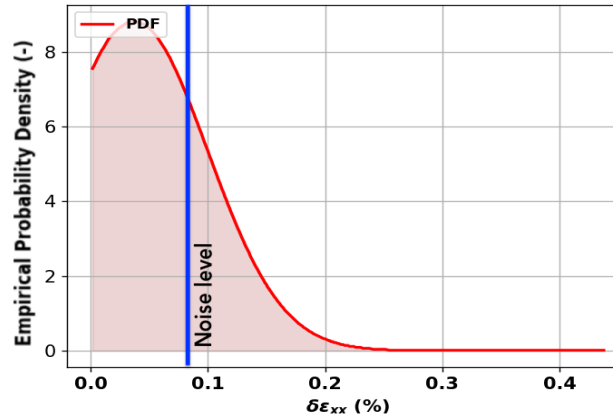
specific orientation, such that grain oriented for single slip do not affect the parameterization of cross slip.

The outcome relies more on the elements with minimal noise and relevance of physical attributes, which mitigates spurious overfitting. Considering the low signal-to-noise ratio in 6, the Rose criterion is widely used by several authors and advises at least a 5:1 ratio for a sound representation [43], it could serve as a filter in the weighting. After introducing an effective noise $\sigma_{\epsilon;DIC}^{\text{eff}} = 5 \cdot \sigma_{\epsilon;DIC}$ in Eq. 6, the points that do not meet the modified Eq. 6 are penalized in the cost function. We recommend to validate the effectiveness of the Rose criterion in the present context of CP parameterization as a next step.

To mitigate partially the noise, several pictures for a same step can be taken and averaging their grey values reduces the noise in the strain field [44]. It implies that the test is ex-situ and taking more pictures at each step of the test brings substantial complexity to the experimental process, especially with high-resolution SEM scans of large field of view.



(a) $\delta\epsilon_{xx}$ distribution with hole and without ROI after modification of the CRSS



(b) $\delta\epsilon_{xx}$ distribution with ROI centered around the hole after modification of the CRSS

Fig. 17: microstructural impact on $\delta\epsilon_{xx}$ after the CRSS variation with the experimental microstructure B, (to compare to Figs. 11b and 11c), (stress-control, 600 MPa)

In addition, other factors prevent a strict match of the measured and calculated strain field. The constitutive law may be too simplistic leading to error and severe overfitting, when applied to other samples. Bertin et al. [45] reported a large residual in the cost-function reaching a constant after several iterations and justifies this by an unadapted CP-model. Experimentally, EBSD scans undergo distortion deforming the grains shape [33] and failed to collect data around the hole (Fig.18), where the microstructure is interpolated. This is problematic, since the most significant information on the strain heterogeneity is concentrated in its vicinity (Fig 10) and its simulated strain value is then questionable due to this microstructural uncertainty. Thus, it is an obstacle for the suggested weighting in the cost-function, as it would mean to maximize the influence of these integration points where the model strain can be biased by the experimental microstructure acquisition.

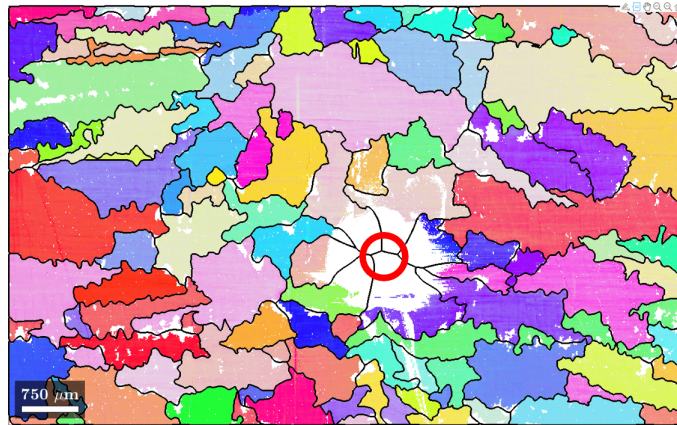


Fig. 18: Raw data from EBSD (microstructure B); the red circle being the actual hole, and the white circle being the area devoid of EBSD data

Most engineering materials are characterized by a high yield strength and have a small plastic region with low hardening slope decoupling the strain from the stress. Thus, a cost function considering only the local strain would not be sufficient to validate the stress values. This added to the above described limitations on the experimental/numerical match, drives to the introduction a part of stress difference in the cost function. An encouraging prospect is the use of DIC coupled with High-Resolution (HR-EBSD) during the mechanical test [12]. This separates the elastic proportion from the total strain. It serves as input to compute the measured local stress that could be incorporated into complex cost-functions weighted between strain and stress measurements. The local stress validation provided by this set-up could give rise to finer understanding of local phenomena controlled by the stress field such as local ratcheting [46].

Conclusion

This study investigated the limitations of DIC in a local validation and calibration based on cyclic tests in the context of fatigue modeling. A necessary criterion comparing strain differences after a parameter variation to the noise from strain measurement with DIC, was employed to assess the limitations of DIC. Overall, this work quantitatively demonstrates that under the low strains of cyclic loading, CP parameter variations induce strain differences consistently below DIC noise levels, which renders DIC-based calibration inherently unreliable in this regime. We further demonstrated after a 20 % CRSS reduction, that:

- Strain parameter sensitivity was maximized for high loads, i.e. far above the yield strength. When below, the strain difference was lower than the standard deviation of strain noise with DIC, for most of the integration points. Therefore, a FEMU calibration on a fatigue test with a low amplitude to capture a cyclic behavior, deteriorates the signal-to-noise ratio. This brings uncertainty to the parameters identification. The coarse uncertainty was evidenced with the necessary criterion, for a more quantitative assessment, we recommend to incorporate artificial noise followed by a comparison of the identified parameter values as in [12, 21].
- Compared to strain-control, mechanical tests under stress-control revealed more favorable to a good strain difference, necessary for the effectiveness of DIC. This effect was specific to the CRSS variation.
- The addition of heterogeneity with a hole in the specimen increased the variability especially around the hole. Therefore, a weighting giving more credit to these elements with high $\delta\epsilon_{xx}$ values or low DIC noise could be included in the cost function as a next step. Increased experimental efforts should be placed on a good quality of the EBSD scan close to the hole.
- The analysis of homogeneous and heterogeneous $\dot{\gamma}_0$ showed that, despite sharing a unique macroscopic stress-strain curve, the DIC could capture the strain differences when the load is high enough. This confirms the result that a macroscale validation is limited. Moreover, the analysis demonstrated that the distribution of $\delta\epsilon_{xx}$ is highly dependent on specific microstructural sample observed (e.g., grain orientation or morphology).

353 Eventually, FEMU is the simplest inverse calibration path. Other identification methods
354 are more complex and challenging like global Integrated-DIC [45], that imposes a FE-form of
355 the measured strain which is more adapted in the case of a low signal-to-noise ratio [36, 47].
356 They could be explored in the context of fatigue modeling.

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.

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367 **Nomenclature**

368 **Acronyms**

369 CP Crystal Plasticity

370 CRSS Critical Resolved Shear Stress

371 DIC Digital Image Correlation

372 EBSD Electron Backscattered Diffraction

373 FCC Face Cubic Centered

374 FEM Finite Element Method

375 FEMU Finite Element Method Updating

376 FIP Fatigue Indicator Parameter

377 HIP Hot Isostatic Pressing

378 HCF High Cycle Fatigue

379 LCF Low Cycle Fatigue

380 PDF Probability Density Function

381 ROI Region of Interest

382 SEM Scanning Electron Microscope

383 **Mathematical operators**

384 : double contraction

385 $sgn()$ signum function

386 **Symbols**

387 C_{11}, C_{12}, C_{44} Cubic Stiffness Parameters

388 E Young's Modulus

389 n Ramberg-Osgood Exponent

390 m Strain Rate Sensitivity Exponent

391 $N_{\text{int.point}}$ Number of integration points

392 K Ramberg-Osgood Constant

393 α Slip system index

394	$\mathbf{M}^\alpha$	Schmid Tensor
395	$\dot{\boldsymbol{\varepsilon}}_p$	Plastic Strain Rate Tensor
396	$\boldsymbol{\varepsilon}$	Strain Tensor
397	$\boldsymbol{\varepsilon}_e, \boldsymbol{\varepsilon}_p$	Elastic, Plastic Strain Tensor
398	$\dot{\gamma}, \dot{\gamma}_0$	Shear Rate, Reference Shear Rate
399	$\boldsymbol{\sigma}$	Stress Tensor
400	σ_y	Yield Stress
401	$\sigma_{\mathcal{E};DIC}$	Noise standard deviation
402	$\mathbb{C}$	Stiffness Tensor
403	τ	Resolved Shear Stress
404	τ_c	Critical Resolved Shear Stress
405	$\delta\boldsymbol{\varepsilon}_{xx}$	Strain difference to a parameter variation

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Appendix A.

Appendix A.1. Link between $\dot{\gamma}_0$ and $\max(M^\alpha)_{\alpha \in \llbracket 1, 12 \rrbracket}$

The aim is to obtain a qualitative trend linking $\dot{\gamma}_0$ to the orientation with the maximal value of the Schmid factor: $\max(M^\alpha)_{\alpha \in \llbracket 1, 12 \rrbracket}$

$\dot{\gamma}_0$ is first expressed in terms of l the mean free path of a dislocation and the density of mobile dislocations ρ_m [38].

$$\dot{\gamma}_0 = \rho_m l b v_G \quad (\text{A.1})$$

with b and v_G two constants, (the Burger vector's norm and a frequency). Considering the approximation at the homogenized scale [38]:

$$l \simeq \rho_m^{-0.5} \quad (\text{A.2})$$

As more plasticity is observed in the highest Schmid factor grains [39], the dislocations density is likewise globally proportional to the maximum value of Schmid factor $\max(M^\alpha)_{\alpha \in \llbracket 1, 12 \rrbracket}$.

$$\rho_m \propto \max(M^\alpha)_{\alpha \in \llbracket 1, 12 \rrbracket} \quad (\text{A.3})$$

Combining Eqs. A.1, A.2 added to the trend in Eq. A.3, provides that:

$$\dot{\gamma}_0 \propto \max(M^\alpha)_{\alpha \in \llbracket 1, 12 \rrbracket} \quad (\text{A.4})$$

Grain	Value of $\dot{\gamma}_0$ in s^{-1}	$\dot{\gamma}_0$ difference (abs. value) (constant-distrib.)
Grain 1	1.56×10^{-6}	9.98×10^{-4}
Grain 2	1.72×10^{-3}	7.20×10^{-4}
Grain 3	2.95×10^{-3}	1.95×10^{-3}
Grain 4	5.95×10^{-6}	9.94×10^{-4}
Grain 5	6.77×10^{-6}	9.93×10^{-4}
Grain 6	6.67×10^{-6}	9.93×10^{-4}
Grain 7	1.58×10^{-6}	9.98×10^{-4}
Grain 8	1.74×10^{-3}	7.40×10^{-4}
Grain 9	2.98×10^{-3}	1.98×10^{-3}
Grain 10	6.42×10^{-6}	9.93×10^{-4}
Grain 11	6.43×10^{-6}	9.93×10^{-4}
Grain 12	6.79×10^{-6}	9.93×10^{-4}
Grain 13	6.43×10^{-6}	9.93×10^{-4}
Grain 14	6.40×10^{-6}	9.93×10^{-4}
Grain 15	6.09×10^{-6}	9.93×10^{-4}
Grain 16	1.54×10^{-6}	9.98×10^{-4}
Grain 17	1.53×10^{-6}	9.98×10^{-4}
Grain 18	1.72×10^{-3}	7.20×10^{-4}
Grain 19	1.74×10^{-3}	7.40×10^{-4}
Grain 20	6.43×10^{-6}	9.93×10^{-4}
Grain 21	1.56×10^{-6}	9.98×10^{-4}
Grain 22	6.87×10^{-6}	9.93×10^{-4}
Grain 23	1.53×10^{-6}	9.98×10^{-4}
Grain 24	2.98×10^{-3}	1.98×10^{-3}
Grain 25	6.88×10^{-6}	9.93×10^{-4}
Grain 26	2.11×10^{-6}	9.97×10^{-4}
Grain 27	2.10×10^{-6}	9.97×10^{-4}
Grain 28	1.63×10^{-6}	9.98×10^{-4}
Grain 29	2.31×10^{-6}	9.97×10^{-4}

Table A.2: Values of $\dot{\gamma}_0$ for each grain for grain labelling correspondance see Fig. A.19

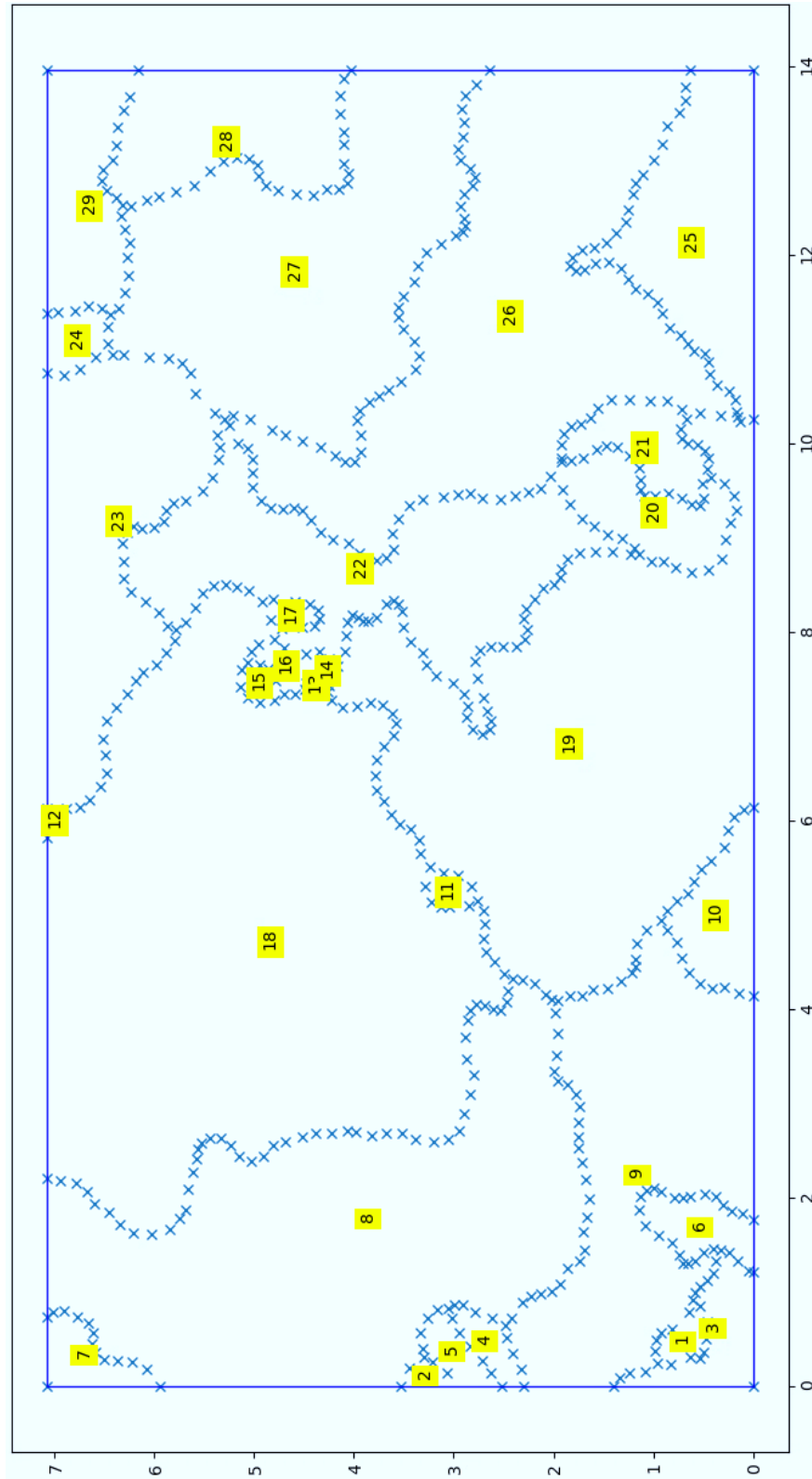


Fig. A.19: Labelling of the grains for the distribution of $\dot{\gamma}_0$



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Robustness of crystal plasticity parameters validation with Digital Image Correlation for fatigue modeling

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