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Intra-grain orientation distributions in deformed aluminium: synchrotron X-ray diffraction experiment and crystal-plasticity finite-element simulation

Loïc Renversade¹ and Romain Quey¹

¹*Mines Saint-Etienne, Univ Lyon, CNRS, UMR 5307 LGF, F - 42023 Saint-Etienne, France*

Abstract

The development of intra-grain orientation distributions is analysed for 446 individual grains of an aluminium polycrystal deformed in tension to successive strains of 1, 1.5, 2, 2.5 and 4.5%. In the experiment, diffraction contrast tomography (DCT) and far-field 3D X-ray diffraction microscopy (3DXRD) were used, and a reduced-order representation of the intra-grain orientation distributions was determined from the broadening of the 3DXRD diffraction spots. A high-resolution finite-element simulation (700 elements/grain on average) was conducted on the same polycrystal, providing detailed information on orientation evolution. Several metrics were considered to analyse the experimental and simulated orientation distributions, including the average disorientation angles and the preferential disorientation axes. The average disorientation angles were found to increase almost linearly with strain, and to be in appreciable correlation between experiment and simulation (albeit evolving faster in simulation). It was shown that the preferential disorientation axes are distributed perpendicular to the tensile direction (Z) and perpendicular to the X–Y component of the Rodrigues orientation vector. Detailed crystal plasticity analyses showed that the distribution of preferential disorientation axes is related to the presence of larger slip variabilities on particular slip systems. Using a simplified approach, it was shown that accurate knowledge of the average stress of a grain is necessary in order to predict the preferential disorientation axis, which is well-captured by the finite-element simulation. The intra-grain stress distribution appears to have comparatively less influence.

1 Introduction

Orientation (or disorientation) distributions develop inside grains of a polycrystal subjected to plastic deformation and are particularly important for practical applications such as industrial rolling, as they influence the mechanical properties [1] and subsequent annealing phenomena such as recrystallization nucleation [2, 3]. From a general point of view, an intra-grain orientation distribution develops depending on the grain attributes (orientation, crystallographic slip systems and slip behavior) and the deformation conditions that the grain undergoes. The deformation is related to the stress, and it is well-known that, in the grains of a deformed polycrystal (and even in deformed single crystals), stress is heterogeneous. Within individual grains, dislocations interact to form cell structures associated to short-range stress heterogeneities, while, across the polycrystal, neighboring grains interact to develop complex long-range stress heterogeneities. Stress heterogeneity inside a grain leads different locations of the grain to undergo different slip activities, which generates different lattice rotations and, in the end, results in the general development of an orientation distribution or, equivalently, a disorientation distribution about the average orientation [4, 5]. Disorientations can be described by disorientation vectors, $\mathbf{r} \theta/2$, where θ are the disorientation angles and \mathbf{r} are the disorientation axes, and, when larger angles develop about particular axes, the disorientation distribution becomes *elongated* in a particular direction or *anisotropic*, or, in other terms, shows a *preferential disorientation axis* [6–8]. From the mechanical point of view, the orientation distributions therefore hold important, archival information on the

slip activity and, more generally, the localization of stress and strain at both grain and intra-grain scales [4]. A recent study also indicated that, when considered at substructure scale, i.e. on populations of dislocation cells, the anisotropy of the orientation distribution provides information on the band structure, which has direct implications on recrystallization nucleation [3]. For more than 20 years, the (full-field) crystal-plasticity finite-element method has been the model of choice to simulate the development of intra-grain orientation distributions inside grains of a polycrystal, as it directly solves for the stress field over the polycrystal and provides the lattice reorientation field resulting from the associated slips [4, 7, 9–11]. In contrast, simpler models (based on simpler localization rules) were mainly developed to predict average grain rotations and the attendant crystallographic texture [12]. While a few early models were developed to reproduce the “orientation splitting” of stable orientations [13, 14], it is only recently that general simplified models have been proposed to predict orientation distribution properties, for example based on phenomenological laws [15] or on second-order micromechanical concepts [4, 5, 16–18]. The micromechanical models, in particular, are built on standard models (Taylor or self-consistent model) to determine the “nominal” state of the grain and then introduce an (intra-grain) stress variability to generate an (anisotropic) orientation distribution [4, 5, 16–18]. As these models describe the material evolution at the intra-grain scale, it is important to validate them against experimental or simulation data obtained at the same scale. Experimentally, this ideally requires observations of the local lattice rotations of individual grains in the bulk of a polycrystal at several steps of a (large) plastic deformation [4, 5]. Finally, the models can also be used to evaluate how different assumptions on the material deformation influence the resulting intra-grain orientation distributions, which both informs on the fundamental behavior of the material and provides inputs for future efforts.

Historically, experimental (local) orientation distributions have been mostly observed in 2-D and after deformation, in single crystals or grains of polycrystals, primarily by electron backscattered diffraction (EBSD) and especially in the case of rolling-type deformation modes [6, 8, 19]. EBSD was also used in conjunction with the “microtexture tracking” or “split sample” technique, by which individual grains are followed on an internal surface of a sample, to access the orientation evolution with strain [20–22]. This allowed comparison with the results of crystal-plasticity finite-element simulations in terms of distribution over all grains or correlation to microstructural attributes, in particular grain (average) orientation [4, 5, 22]. Actual 3-D analyses, which allow for direct, grain-by-grain comparison between experiment and simulation, became possible with the advent of high-energy X-ray diffraction techniques, which have been applied mainly to uniaxial loadings [23]. This has led to the so-called “far-field 3-D X-ray diffraction microscopy (3DXRD)” technique [24], which was first applied to follow the average rotations of grains in a plastically-deformed aluminium polycrystal [25] and compare them to predictions from simple models [26]. Derivative techniques were then developed to access intra-grain orientation information, such as diffraction-contrast tomography (DCT and 6D-DCT) [27, 28], which primarily facilitates mapping of undeformed or slightly deformed polycrystalline microstructures ($\varepsilon < 5\%$), or high-energy diffraction microscopy (HEDM) [29], which also applies to moderately deformed polycrystalline microstructures ($\varepsilon < 20\%$). Applications include Refs. [30, 31]. However, the 3DXRD technique itself, which is experimentally simpler, also provides some degree of information on intra-grain orientation distributions [32]. Standard applications, which focus on the determination of the average orientations of grains, use only the average positions of the spots, but their broadening contains information on the orientation distributions (excluding the spatial arrangements), which can be used for example to determine the complete ODF of a deformed grain [33, 34], or directly compare experiment and simulation [35]. When the focus is specifically on the anisotropy properties of the orientation distributions, it should also be possible to determine them directly from the broadening of the diffraction spots.

In this work, an experiment based on DCT and 3DXRD is used to track the development, via the broadening of the diffraction spots, of the intra-grain orientation distributions in the grains of a deformed polycrystal subjected to tension, and the results are compared to those of a simulation based on the crystal-plasticity finite-element method. Using both data sets (and a simplified model), the goal is to develop a better understanding of the development of the intra-grain orientation distributions. The paper proceeds as follows. First, the experiment and the method to determine the properties of the intra-grain orientation distributions

from the observed diffraction spots are presented in Section 2. Then, the finite-element simulation and the procedure to determine the same properties are presented in Section 3. Next, the results on different metrics are presented and compared in Section 4. Section 5 relates the metrics, in particular the preferential disorientation axes, to deformation mechanisms, using the simplified model. Section 6 completes the paper with conclusions.

2 Experiment

A high-purity Al–0.3wt% Mn alloy was used. After casting, the material was cold-rolled to 80% height reduction. A flat, dog-bone specimen was spark-machined with its tensile axis along the rolling direction, and with a gauge of section 1 mm \times 1 mm and height 1.5 mm. The material was then recrystallized at 450 °C for 25 min. This resulted in a microstructure consisting of nearly equiaxed grains of uniform orientations and an average size of about 150 μ m, with only a relatively limited crystallographic texture. The grain orientations and reorientations developing as the specimen was subjected to plastic deformation were then observed *in situ* by high-energy X-ray diffraction at the Materials Science beamline of ESRF (ID11).

2.1 DCT and 3DXRD observation

Before deformation, the polycrystal structure of the full gauge section of the specimen was mapped by DCT [36], see Figure 1a. This was done using a beam of energy 41.7 keV and a FReLoN camera with 2048 \times 2048 pixels of an effective size of 1.4 μ m, located 5 mm behind the sample. The X-ray beam was 1 mm wide and 550 μ m high, so that three DCT scans were carried out along the loading direction to map the polycrystal structure in a total region of height 1.4 mm. An overlap of 75 μ m was used between adjacent scans to ensure a continuous mapping of the polycrystal structure and later facilitate the merging of the acquired volumes into the single, final volume representing the polycrystal structure of the full gauge section. The acquisition of each volume was done over a full sample revolution, with an integration step of 0.1° (3600 diffraction images) and an exposure time of 1 s. To merge the three volumes, registration was used to minimize the difference between the polycrystal structures within the overlapping regions. The grains at the overlap between two volumes were identified manually and merged automatically in the final volume.¹ In the final volume, the average orientations of the grains obtained by merging were computed from the orientations they had in the initial volumes, by simple orientation averaging, which did not imply changes of more than 0.05°. The resulting polycrystal volume contained 1848 grains and is shown in Figure 1b and its texture in Figure 1c.

Deformation was then applied using the Nanox load frame [37], in several steps, to successive strains of 1, 1.5, 2, 2.5 and 4.5% (measured at the gauge section). After each deformation step, the grain orientations were measured by 3DXRD at the center of the gauge section, on a height of 550 μ m [23]. This was done using a beam of energy 60 keV and a FReLoN camera with 2048 \times 2048 pixels of an effective size of 48.5 μ m, located 260 mm behind the sample. Up to the strain of 2%, a beam of height of 550 μ m and width of 1 mm was used, and the acquisition was done over a full sample revolution, with an integration step of 0.03° (12,000 diffraction images) and an exposure time of 0.03 s. At higher strains, the acquisition parameters had to be adapted, due to the peak broadening resulting from plastic deformation, to avoid spot overlaps and excessive intensity loss. At a strain of 2.5%, the beam height was reduced to 275 μ m, and two adjacent scans were acquired with an integration step of 0.06° (6000 diffraction images). At a strain of 4.5%, the height was reduced to 185 μ m, and three adjacent scans were acquired with an integration step of 0.2° (1800 diffraction images) and an exposure time of 0.06 s. Standard post-processing was used to “index” the diffraction spots and relate them to the corresponding grains. The set of analysed grains is shown on Figure 1d, and typical orientation spots are provided in Figure 1e. Diffraction spots are inherently 3-D intensity distributions, but are acquired as a set of 2-D detector images (in u – v directions) at fixed rotation angle (ω). For each spot,

¹This was done before the dilation step of the standard DCT post-processing procedure.

a stack of detector images can be used to reconstruct the full distribution. The distribution can then be projected into the azimuthal plane (η, ω) to retain only the lattice rotation information [23]. Only the spots that do not overlap with the spots of other grains were considered, which lead to sets of between 40 and 100 spots for each grain and at each strain. The resulting number of available spots tended to decrease as strain increased, but always remained higher than about 40 (which is sufficient to unambiguously and accurately determine the anisotropy properties of the corresponding orientation distribution). Among the total of 824 grains contained in the region covered by 3DXRD, 466 grains (arbitrarily located in the 3DXRD region) could be followed during the entire deformation and will be used in the following.

As can be seen in Figure 1a, the microstructure was initially mapped (by DCT) in a region significantly larger than the region in which grains were then tracked during deformation (by 3DXRD), with region heights of 1.4 mm and 550 μm , respectively. This allows to know the neighborhood of the analysed grains, over several grain lengths, which is particularly important since the deformation of a grain depends not only on its own attributes (especially orientation) but also on the mechanical interaction with its neighbors. In the simulation (Section 3), the deformation will be applied to the polycrystal defined over the DCT region (instead of only the 3DXRD region), which will ensure that all the grains of the analysis region deform under the same conditions as in the experiment.

2.2 Determination of the intra-grain disorientation distributions

The disorientation distribution of a grain can be expressed in tangent space of orientation space, where a disorientation vector, \mathbf{w} , is defined as $\mathbf{w} = \mathbf{r}\theta/2$, where \mathbf{r} and θ are the disorientation axis (expressed in the reference coordinate system²) and disorientation angle, respectively [38]. In that space, the disorientation distribution of a grain is typically *unimodal* and *anisotropic* [4, 6], and it will also be the case in this work. Such a distribution clusters about the origin of the space (which represents the average orientation), extends differently depending on the direction and typically shows bell-shaped frequency profiles (when going across the distribution) that approach a normal distribution [4, 19], as exemplified in Figure 2. In contrast, multimodal orientation distributions (that cluster about a small number of distinct orientations) are only observed for grains of specific initial orientations deformed to large plastic strains, while these grains would still develop a unimodal orientation (or disorientation) distribution at small strains [5, 22]. In this work, we are only interested in the (statistical) anisotropy properties of the orientation distributions and therefore will determine them directly from the diffraction spots, with no regards to the actual shapes of the distributions. For each grain, the diffraction spots (described in azimuthal plane (η, ω)) correspond to intensity maps, I_{exp} , which represent the input data of the approach.

2.2.1 Principle

For each grain, a reduced-order representation of the disorientation distribution is considered, and its parameters are determined from the set of intensity maps (I_{exp}). Formally, this corresponds to the process of fitting an analytical function to a collection of discrete data points, but with the analytical function and the discrete data points defined in different spaces.

Consistent with the distribution properties described previously, the disorientation distribution is defined as a 3-variate normal distribution, P ,

$$P(\mathbf{w}) = \prod_{i=1}^3 \frac{1}{\sqrt{2\pi}\theta_i} \exp\left(-\frac{(\mathbf{w} \cdot \mathbf{v}_i)^2}{2\theta_i^2}\right), \quad (1)$$

where \mathbf{v}_i are the three (orthogonal) principal directions of the distribution and θ_i are the associated characteristic lengths of the distribution ($\theta_1 \geq \theta_2 \geq \theta_3$). This function combines the different rotation trends (θ_i) in

²Throughout the article, “reference coordinate system” refers to the system of axes attached to the sample, (X, Y, Z), also called “reference frame” or “sample frame” in the literature.

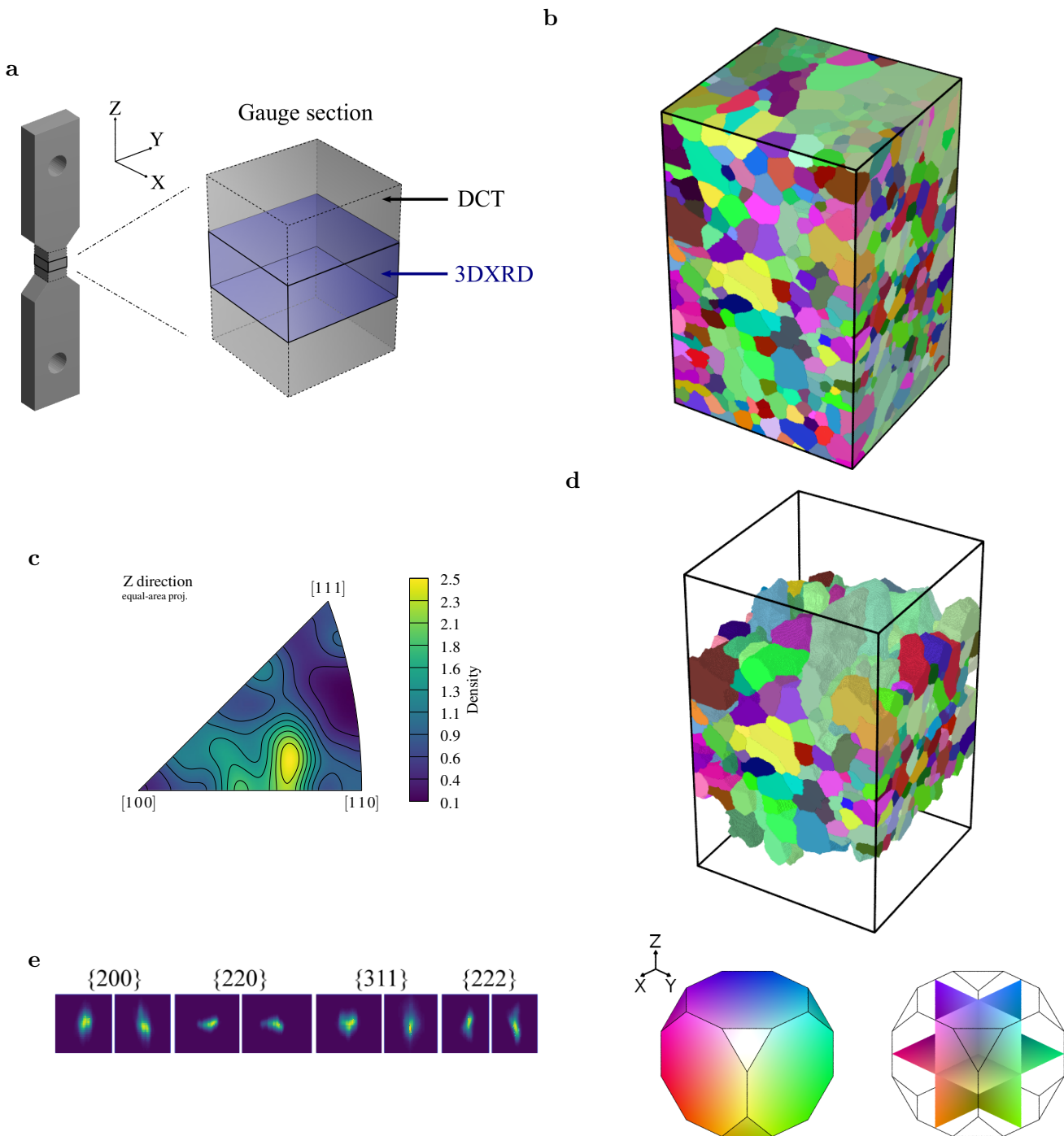


Figure 1: High-energy X-ray synchrotron experiment. (a) Tensile specimen and observed regions in DCT and 3DXRD, (b) initial microstructure obtained by DCT and colored by orientation, (c) crystallographic texture on the standard triangle (computed from the 466 followed grains), (d) grains followed by 3DXRD, and (e) example of a series of diffraction spots of a particular grain (azimuthal projection, $\varepsilon = 4.5\%$). (b) and (d) are colored by orientation as shown by the Rodrigues space color key.

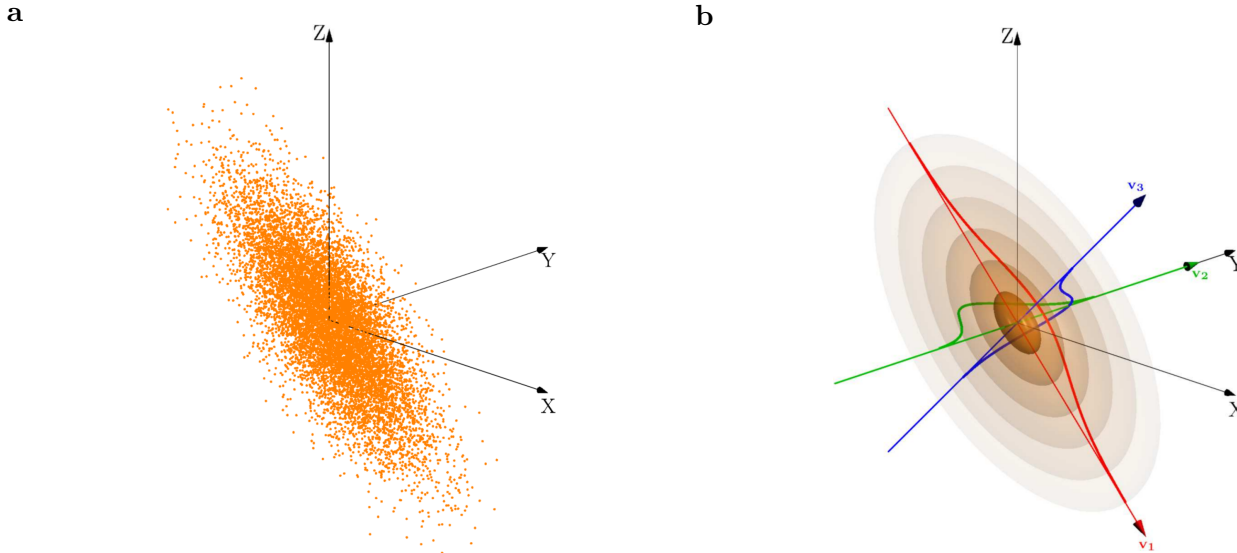


Figure 2: Typical disorientation distribution of a deformed grain, plotted in tangent space of orientation space ($\mathbf{r} \theta/2$ vectors). (a) Set of 10,000 randomly-generated disorientations, and (b) corresponding frequency distribution (P), of principal axes \mathbf{v}_i , $i = 1, 2, 3$. The (ellipsoidal) surfaces represent isovalues of the distribution, and the curves along the three axes are the frequency profiles, which are normal distributions of standard deviations θ_i . The case of $\theta_1 = 0.0087$ ($\simeq 1^\circ$) and $\theta_2 = \theta_3 = 0.0044$ ($\simeq 0.5^\circ$) is represented.

three dominant (principal) directions (\mathbf{v}_i) to finally lead to a general, anisotropic distribution. Figure 2b provides an example of such a distribution. By definition, P is centered on the origin of the space and integrates to 1 over the full space. The first principal axis (\mathbf{v}_1 , associated to θ_1) corresponds to the disorientation axis about which the disorientation angles are the highest and will be referred to as “preferential disorientation axis” in the following [4].

The parameters of the disorientation distribution (\mathbf{v}_i and θ_i) are determined using a method based on the generation of a set of diffraction spots, of intensities I_{gen} , from the disorientation distribution (often referred to as “forward simulation”³), and the optimization of its parameters so as to reproduce the set of experimental diffraction spots (I_{exp}) as closely as possible. First, initial \mathbf{v}_i and θ_i values are considered: $\theta_{1,2,3}$ are set to $\delta\omega$ (the integration step of the 3DXRD scan), and $\mathbf{v}_{1,2,3}$ are simply set to be coincident with the axes of the reference coordinate system. Then, iterations are carried out on the values of \mathbf{v}_i and θ_i (and so, on the disorientation distribution as a whole), until convergence, with these steps:

1. From \mathbf{v}_i and θ_i , generate diffraction spots, I_{gen} ;
2. From the experimental and generated diffraction spots (I_{exp} and I_{gen}), compute their correspondence, r (correlation factor defined in the following);
3. From the evolution of r over iterations (i.e., as a function of \mathbf{v}_i and θ_i), modify \mathbf{v}_i and θ_i values so as to maximize r .

Final results are values of \mathbf{v}_i and θ_i , and therefore the disorientation distribution (P) corresponding to the set of intensity maps (I_{exp}) of a particular grain.

The generation of diffraction spots (item 1) is described in Section 2.2.2, while the spot comparison (item 2) is defined in Section 2.2.3 and optimization (item 3) is described in Section 2.2.4. An example of application is provided in Section 2.2.5.

³In this article, the expressions “forward simulation” or “simulation” are not used to refer to the generation of diffraction spots to avoid confusion with the (finite-element) simulation.

2.2.2 Generation of diffraction spots from the reduced-order disorientation function

Given values of \mathbf{v}_i and θ_i (which define P), diffraction spots (to be compared to the experimental ones) are generated by first considering a “discrete approximation” of P , as illustrated on Figure 3. At small plastic strains, for which lattice rotations are limited, P is mostly contained within a small region about the origin of tangent space, and its discrete approximation can appropriately be defined in this region. This region was taken as a cube of half edge length equal to $3\theta_1$ (the greatest “three standard deviations”) to effectively contain most of the distribution, with N voxels along each direction. A value of $N = 80$ provided a good balance between the discretization accuracy and the computation time associated to the generation of the spots from the orientation distribution (which scales with N^3). The discrete approximation of P can then be processed as a set of weighted disorientations $\{(\mathbf{w}^\alpha, \phi^\alpha), \alpha = 1, \dots, N^3\}$, where the disorientations (\mathbf{w}^α) correspond to the centers of the voxels of the region, and the weights (ϕ^α) correspond to their P values ($\phi^\alpha = P(\mathbf{w}^\alpha)$).

From the grain average orientation and the discretized disorientation distribution ($\{\mathbf{w}^\alpha, \phi^\alpha\}$), an orientation set, $\{(\mathbf{q}^\alpha, \phi^\alpha)\}$, was generated, and the diffraction spots corresponding to its (hkl) reflections were then computed. For a given (hkl) , the diffraction spot was obtained in (η, ω) coordinates as the sum of the intensities (ϕ^α) contributed by all orientations (\mathbf{q}^α), at specific locations $(\eta^\alpha, \omega^\alpha)$, resulting in an intensity map, I_{gen}^0 . For each orientation (\mathbf{q}^α), ω^α was determined from the Laue equation, while η^α was obtained via the diffraction vector, \mathbf{g}_L , which is given by the standard forward projection relation,

$$\mathbf{g}_L = \boldsymbol{\Omega}_\omega \mathbf{U}^{-1} \mathbf{B} \begin{pmatrix} h \\ k \\ l \end{pmatrix}, \quad (2)$$

where $\boldsymbol{\Omega}_\omega$ represents the rotation of angle ω^α about the sample rotation axis, \mathbf{U} the crystal orientation, and \mathbf{B} the orthogonalization matrix [23, 29]. The orientation weight (ϕ^α) was then simply added to the intensity of the corresponding bin of the (η, ω) grid. However, the resulting map (I_{gen}^0), generated only from the discrete approximation of the disorientation distribution, does not include the effects of other microstructural or experimental factors that affect the experimental intensity map (I_{exp}). These effects must therefore be taken into account to lead an unbiased comparison of the experimental and generated intensity maps, and this can be done by “adding” them to the generated intensity maps. The first operation is related to the ODF discretization and the “sharp” integration of the intensities of the diffraction vectors (as Dirac delta functions, i.e. independently of the distance to the bin center or the distance to the centers of the neighboring bins) and introduces “smoothing”, with a typical characteristic length equal to the bin size, which is similar to an experimental “broadening effect” of the detector itself. The second operation introduces a “grain size effect”, which causes broadening along η , directly related to the grain size. The actual generated intensity map, I_{gen} , was therefore obtained as

$$I_{\text{gen}}(\eta, \omega) = I_{\text{gen}}^0(\eta, \omega) \circ G_1(\eta, \omega) \circ G_2(\eta), \quad (3)$$

where \circ is the convolution product. The ODF discretization correction, $G_1(\eta, \omega)$, is defined as

$$G_1(\eta, \omega) = \frac{1}{\sqrt{2\pi}\delta r^2} \exp\left(-\frac{\eta^2 + \omega^2}{2\delta r^2}\right), \quad (4)$$

where δr is the bin size of the (η, ω) grid. The grain size effect, $G_2(\eta)$, is defined as

$$G_2(\eta) = \frac{1}{\sqrt{2\pi}r_i^2} \exp\left(-\frac{\eta^2}{2r_i^2}\right), \quad (5)$$

where r_i is the grain equivalent radius (determined by DCT or, equivalently, by 3DXRD, using the average spot intensity of the grain [39]) expressed in units of η . An example of generated diffraction spot is provided in Figure 3b.

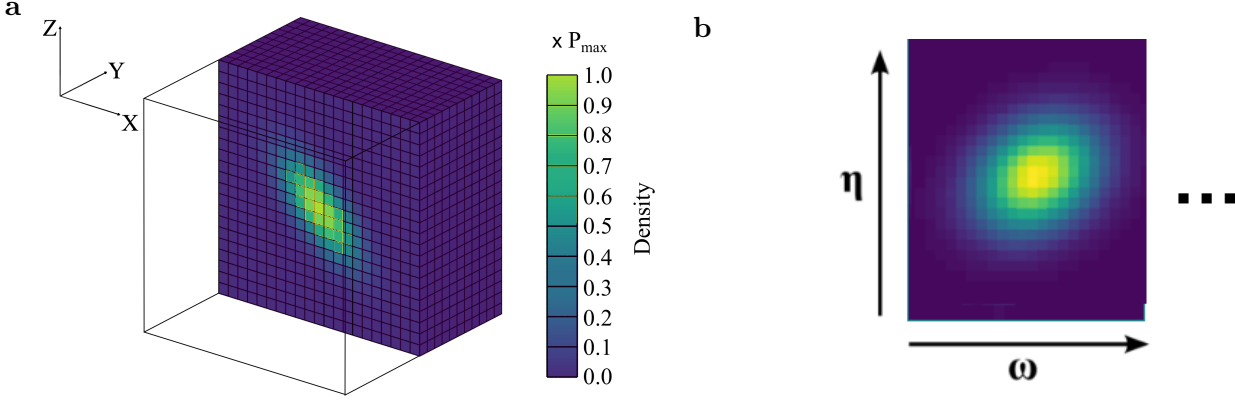


Figure 3: Discrete approximation of the disorientation distribution (P) of a grain, and example of corresponding diffraction spot. The distribution shown on Figure 2b is used. (a) Discretized approximation of P in a region of size $\Delta r = 0.0524$ ($\simeq 6^\circ$) with $N = 23$, resulting in $\delta r = 0.0022$ ($\simeq 0.25^\circ$) and a total of 12,167 voxels (in practice, $N^3 = 512,000$ voxels are used). (b) Corresponding intensity map in the (η, ω) plane (I_{gen}).

2.2.3 Correspondence between experimental and generated diffraction spots

The correspondence between an experimental spot and a generated spot is quantified by the Pearson product-moment correlation coefficient, r , which is defined as

$$r = \frac{\sum_{i,j} (I_{\text{exp}}^{ij} - I_{\text{exp}}) (I_{\text{gen}}^{ij} - I_{\text{gen}})}{\sqrt{\sum_{i,j} (I_{\text{exp}}^{ij} - I_{\text{exp}})^2} \sqrt{\sum_{i,j} (I_{\text{gen}}^{ij} - I_{\text{gen}})^2}}, \quad (6)$$

where (i, j) loops over all bins, I_{\bullet} is the average of I_{\bullet}^{ij} over all bins, and r reaches the maximal value of 1 for a perfect linear correlation. The correlation coefficient (r) is insensitive to the difference in average values, so that the generated spots do not have to be defined by actual intensities. The objective function (to maximize) is then simply expressed as

$$r = \frac{1}{N} \sum_{k=1}^N r_k, \quad (7)$$

where N is the number of diffraction spots.

2.2.4 Optimization

While the set of principal axes (\mathbf{v}_i) and characteristic length (θ_i) represent a total of 12 variables, the principal axes (\mathbf{v}_i) form a coordinate system whose orientation with respect to the reference coordinate system can be described by a (3-D) Rodrigues vector, thereby reducing the total number of variables from 12 to six. Determining the values of the six variables so as to maximize r consists of a non-linear optimization problem, of unknown gradient, which is solved using the local optimization algorithm Subplex of the NLOpt library [40, 41]. The Subplex algorithm is derived from the Nelder-Mead simplex algorithm and decomposes high-dimensional problems into a series of low-dimensional problems that can be handled by the simplex algorithm.

2.2.5 Example of grain 1212

The method is applied to a particular grain (grain 1212), of an average size of 60 μm and an arbitrary orientation (26° away from Cube). For this grain, 91 spots at $\varepsilon = 1\%$ down to 47 spots at $\varepsilon = 4.5\%$ were

obtained from the experimental data. The evolution of eight spots that were available at all deformations is showcased in Figure 4, and some of their anisotropy properties and r value are provided in Table 1. It can be clearly seen that, as deformation accumulates, the experimental diffraction spots broaden and show different elongated shapes depending on the (hkl) direction, but also depending on the strain, which indicates that the anisotropy properties of the orientation distribution evolve during deformation. The generated spots properly capture the size, shape and direction of the experimental spots at all strains. Clearly, they also “simplify” the experimental spots, which are less regular and sometimes exhibit local fluctuations, but the differences can be considered of second order relative to the global, anisotropic character of the distribution. Some degree of fluctuation, in particular, may be associated to experimental noise, which the reduced-order representation allows to “filter”. For the grain of interest, the correlation coefficient (r) increases with strain to a value as high as 0.95 at $\varepsilon = 4.5\%$, which tends to confirm that 3-variate normal distributions can be used to represent the orientation distributions of grains deformed to a plastic strain of a few percents [19].

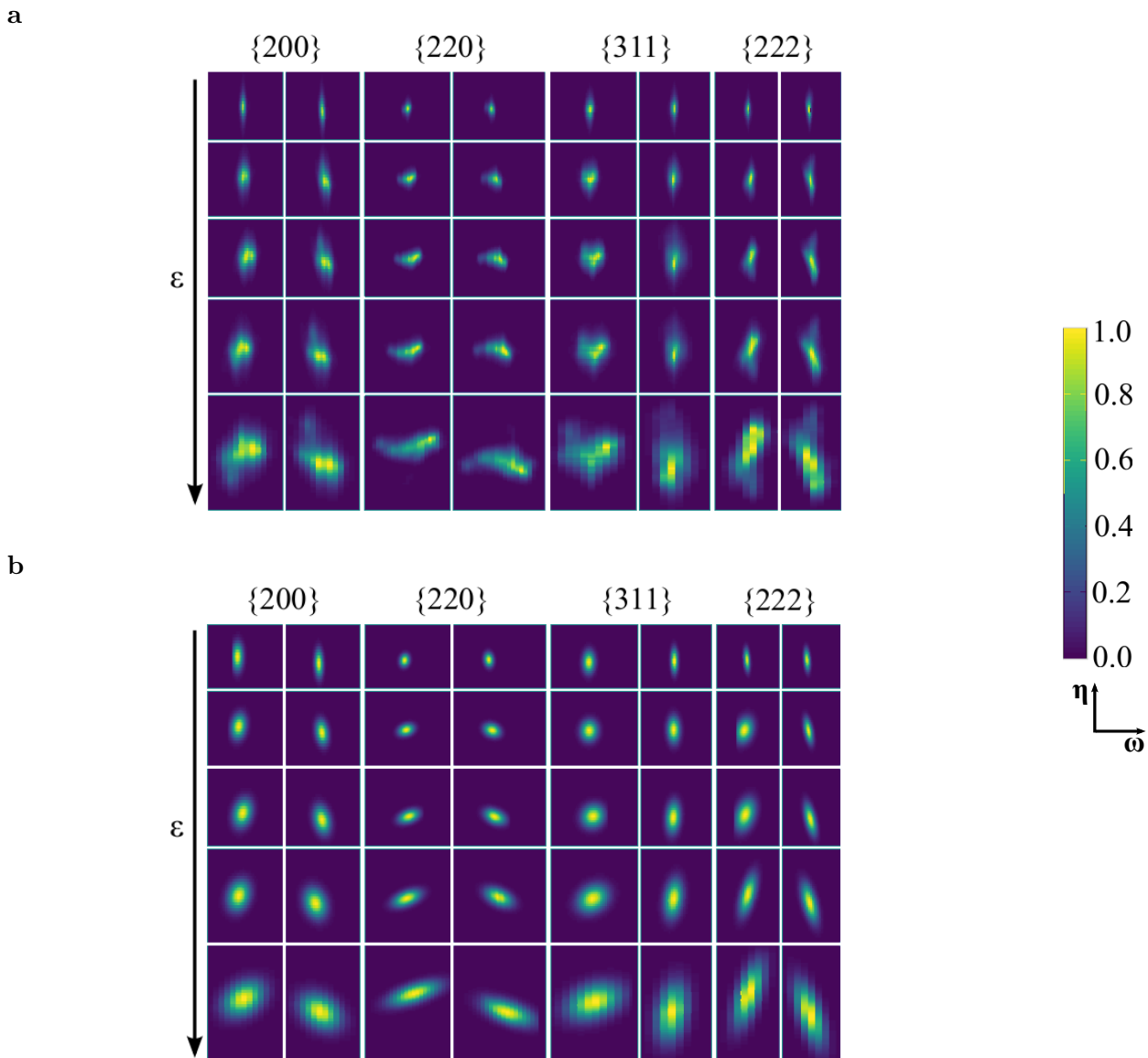


Figure 4: Comparison between experimental and generated spots for an arbitrary grain (grain 1212): (a) experimental and (b) generated. The spots are arranged by types of reflection (horizontally) and strain levels (vertically), and are normalized to a maximal intensity of 1. The (hkl) directions are (200) , $(\bar{2}00)$, (220) , $(2\bar{2}0)$, $(31\bar{1})$, $(\bar{1}\bar{3}\bar{1})$, $(2\bar{2}2)$ and $(\bar{2}2\bar{2})$, from left to right, and the successive strains are $\varepsilon = 1, 1.5, 2, 2.5$ and 4.5% .

Table 1: Assessment of intra-grain orientation distributions: results of the optimization approach for an arbitrary grain (grain 1212). \mathbf{v}_1 is expressed in the reference coordinate system.

Strain	Number of spots	θ_1 (°)	θ_2 (°)	θ_3 (°)	\mathbf{v}_1	r
1.0%	91	0.08	0.04	0.02	(0.836, 0.119, -0.536)	0.80
1.5%	83	0.16	0.08	0.05	(0.936, 0.194, -0.292)	0.86
2.0%	78	0.22	0.09	0.07	(0.946, 0.147, -0.288)	0.88
2.5%	44	0.30	0.13	0.09	(0.963, 0.050, -0.266)	0.93
4.5%	47	0.56	0.25	0.15	(0.962, 0.060, -0.267)	0.95

3 Simulation

The plastic deformation of the polycrystal was simulated over the region mapped by DCT (1848 grains) in order to predict the resulting lattice reorientations of the grains, and the results of the 466 grains followed by 3DXRD were used for the analysis. Having a simulation region (the DCT region) significantly larger than the analysis region (the 3DXRD region) made it possible to consider the real neighbors of the grains of the analysis region and to apply the boundary conditions sufficiently far from these grains not to affect their reorientations. The polycrystal deformation was simulated using the crystal-plasticity finite-element method, in which the grains of the polycrystal are discretized into finite elements, deform by slip on specific crystallographic systems, and interact according to mechanical equilibrium to develop heterogeneous stress and strain fields. The free / open-source software packages Neper and FEPX were used for the polycrystal meshing, parallel simulation deformation and result post-processing [11, 42, 43].

3.1 Constitutive equations

Plastic deformation occurs by slip on the 12 $\{111\}\langle 110\rangle$ systems. The slip rate of a given slip system, $\dot{\gamma}^\alpha$, is related to its resolved shear stress, τ^α , through a power law,

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^{\frac{1}{m}} \text{sgn}(\tau^\alpha), \quad (8)$$

where $\text{sgn}(x) = 1$ if $x \geq 0$ and $\text{sgn}(x) = -1$ if $x < 0$, m is the strain-rate sensitivity coefficient, $\dot{\gamma}_0$ is the fixed-state strain rate scaling coefficient, and g^α is the current system strength. The hardening on a slip system, \dot{g}^α , is described by a Voce hardening assumption,

$$\dot{g}^\alpha = h_0 \left(\frac{g_s - g^\alpha}{g_s - g_0} \right)^n \dot{\gamma}, \quad \text{where } \dot{\gamma} = \sum_{\alpha} |\dot{\gamma}^\alpha|. \quad (9)$$

At the initial state ($\varepsilon = 0$), all g^α are taken equal to the g_0 value. In such a case, it can be noticed from Equation 9 that the yield surface grows isotropically with strain. To identify the slip parameters, the (experimental) stress-strain curve of the material was measured on a sample deformed at the laboratory, and simulations were carried out on a 1000-grain polycrystal with random grain orientation (consistent with the weak texture of the material). The slip parameters were adjusted in the simulation until a good fit between the experimental and simulated stress-strain curves was obtained, which lead to values of $\dot{\gamma}_0 = 1 \text{ s}^{-1}$ (a convention), $m = 0.03$, $h_0 = 47 \text{ MPa}$, $g_0 = 6 \text{ MPa}$, $g_s = 455 \text{ MPa}$ and $n = 2.6$. The (macroscopic) stresses measured during the 3DXRD experiment happened to be slightly smaller, but this was properly reproduced by the finite element simulation (using the same slip parameters) and can be attributed to the presence of texture in the DCT/3DXRD sample (Figure 1c). The stress-strain curves are provided in Figure 5. The crystal elastic anisotropy was modeled using stiffness parameters of $C_{11} = 107.3 \text{ GPa}$, $C_{12} = 60.9 \text{ GPa}$ and $C_{44} = 56.6 \text{ GPa}$ [44]. A complete description of the constitutive model and the finite element method implementation can be found in Refs. [9, 10].

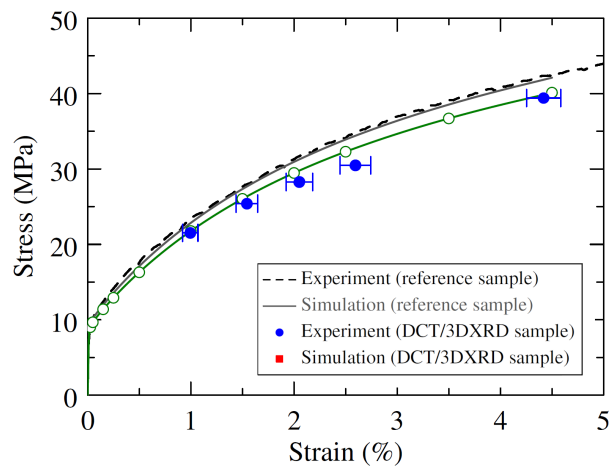


Figure 5: Macroscopic stress-strain curves in experiment and simulation. The reference sample was deformed at the laboratory and used to determine the slip parameters.

3.2 Polycrystal meshing and deformation

The polycrystal image obtained by DCT was defined in raster format, using voxels. In contrast, the synthetic polycrystals typically used in finite-element crystal-plasticity simulations are defined in vector format, using points, straight edges, planar faces and (convex) volumes, which is the input of standard meshing tools [42, 45]. In this work, such a description was accordingly obtained by approximating the polycrystal image by its nearest convex-grain geometry, using the general approach presented in Ref. [43]. Formally, any polycrystal made of convex grains which meet along grain boundaries, triple lines and quadruple points, such as the polycrystal used in this work but also most single-phase (and some multi-phase) polycrystals, corresponds to a normal tessellation, and any normal tessellation can be represented by a Laguerre tessellation [46]. It is therefore possible to approximate a polycrystal by an optimal convex-cell geometry using a Laguerre tessellation, given proper determination of its parameters.

Given a spatial domain $D \in \mathfrak{R}^n$, a Laguerre tessellation is defined from a set of seeds, S_i , described by their positions, \mathbf{x}_i , and weights, w_i , where each seed (S_i) generates a Laguerre cell, C_i , as follows:

$$C_i = \left\{ P(\mathbf{x}) \in D \mid d(\mathbf{x}, \mathbf{x}_i)^2 - w_i < d(\mathbf{x}, \mathbf{x}_j)^2 - w_j \quad \forall j \neq i \right\}, \quad (10)$$

where d is the Euclidean distance. In 3-D, and under the Laguerre tessellation parameterization, any normal tessellation comprising N cells (and so any polycrystal made of N convex grains) can therefore be described by a set of a maximum of $4N$ parameters. It is, however, non trivial to determine the values of these parameters. In this work, this was done by minimizing an objective function, O , that quantifies the difference between the input (DCT) polycrystal and the output (convex-cell) tessellation in terms of distance between their internal boundaries [43],

$$O = \sqrt{\frac{2}{n_v \langle d \rangle^2} \sum_{i=1}^N \sum_{v_k \in G_i^b} d(v_k, C_i)^2} \quad \text{with} \quad n_v = \sum_{i=1}^N |G_i^b|, \quad (11)$$

where G_i^b represents the set of boundary voxels of grain i , $d(v_k, C_i)$ is the Euclidean distance between a boundary voxel of grain i , $v_k \in G_i^b$, and its corresponding cell, C_i , $|G_i^b|$ is the number of elements of G_i^b , n_v is the total number of boundary voxels, and $\langle d \rangle$ is the average grain size [43].⁴ The optimization problem is large-scale, non-linear and of unknown gradient, and was solved using the local optimization algorithm Subplex of the NLOpt library [40, 41, 43]. The final average distance between the grain boundaries of the polycrystal and those of the approximating tessellation was 10 μm .

The cells were then assigned the crystal orientations of the grains, and the tessellation was regularized so as to remove its smallest edges and faces, which avoids the generation of low-quality elements during meshing [42]. The tessellation was finely and homogeneously discretized into 10-node tetrahedral elements, with an average of 700 elements per grain, which lead to a mesh comprising about 1,338,000 elements and 1,833,000 nodes. The experimental polycrystal, approximating tessellation and final mesh are shown in Figure 6a-c (the approximations are simply related to the experimental grain non-convexities).

The mesh was subjected to the experimental deformation of 4.5% tension (at a strain rate of 10^{-2} s^{-1}) by imposing a non-zero z velocity to the top surface while the bottom surface remained fixed along z (with additional constraints to avoid rigid body motions). Figure 6d provides an example of results on the deformed mesh.

3.3 Determination of the intra-grain disorientation distributions

For each grain (and at each strain), the finite-element simulation provides a set of weighted orientations (corresponding to the elemental orientations and volumes), $\{(\mathbf{q}^\alpha, \phi^\alpha), \alpha = 1, \dots, N\}$, from which the

⁴The expression differs from the one used in Ref. [43] by a scaling factor, but this does not affect the optimization nor final tessellation.

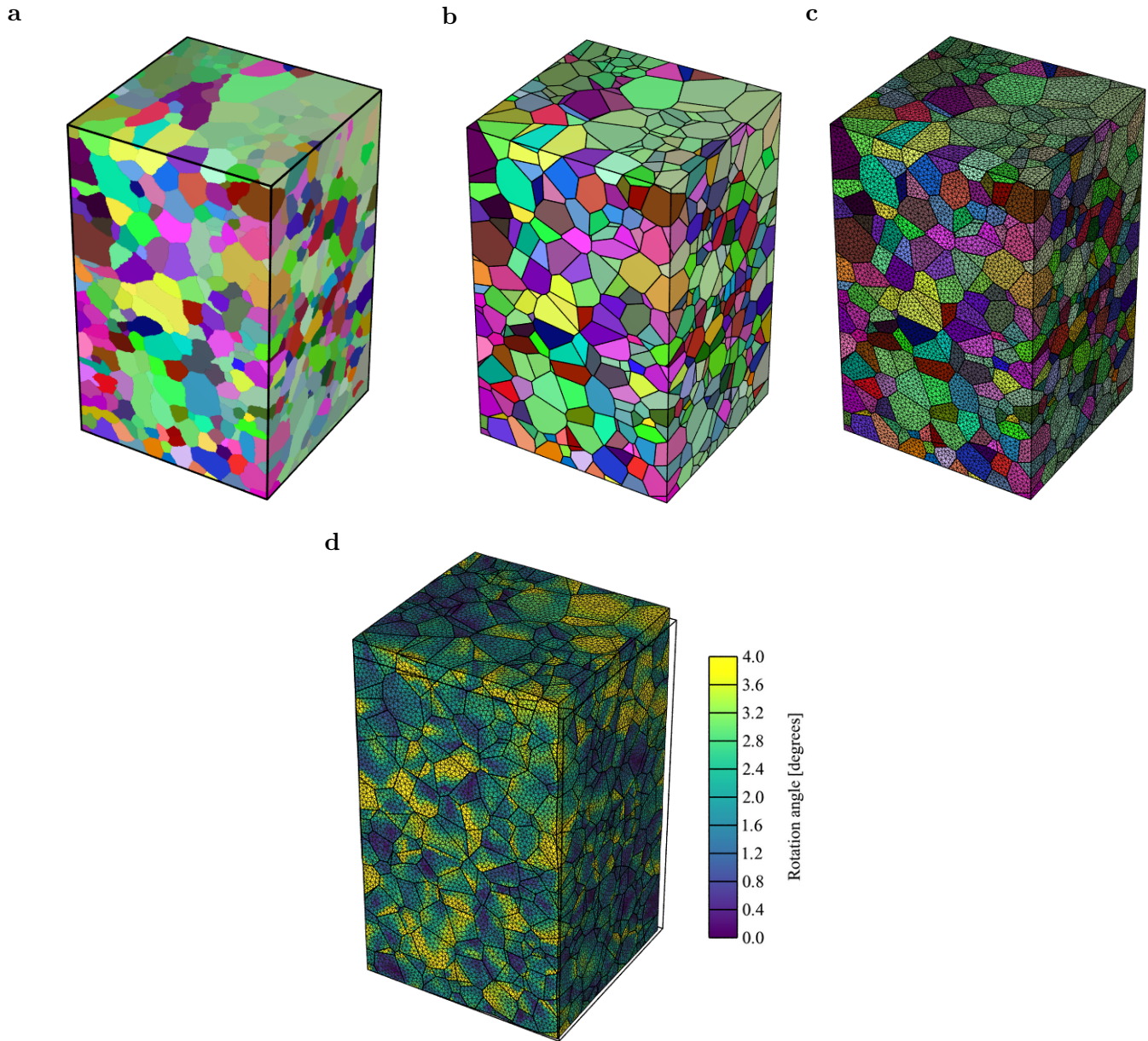


Figure 6: Mesh generation from the DCT polycrystal and first results of the finite-element simulation. (a) DCT polycrystal (same as Figure 1a), (b) approximating tessellation, (c) finite element mesh, and (d) lattice rotation angle (from the initial orientation) at 4.5%. Note the good agreement between experiment and simulation for both samples. (a–c) are colored by orientation as in Figure 1.

anisotropy parameters \mathbf{v}_i and θ_i of the disorientation distribution can be determined. The average grain orientation, $\bar{\mathbf{q}}$, is first computed by quaternion averaging [4,6]. For each element of the grain, the disorientation with respect to the average orientation is then computed and written as the disorientation vector, \mathbf{w}^α (associated to its weight, ϕ^α).

The anisotropy parameters of the discrete disorientation distribution can then be computed directly (i.e., without actually fitting the distribution⁵), as first proposed by Glez and Driver [6] for EBSD data and Barton and Dawson [7] for crystal-plasticity finite-element data, as illustrated in Figure 7. Given the set of weighted disorientations expressed in tangent space, $\{(\mathbf{w}^\alpha, \phi^\alpha), \alpha = 1, \dots, N\}$, a 3×3 covariant matrix, \mathbf{S} , is defined as

$$\mathbf{S} = \frac{1}{\Phi} \sum_{\alpha=1}^N \phi^\alpha (\mathbf{w}^\alpha \otimes \mathbf{w}^\alpha) \quad \text{with} \quad \Phi = \sum_{\alpha=1}^N \phi^\alpha, \quad (12)$$

which is symmetric and can be diagonalized. The eigenvectors and the square roots of the eigenvalues of \mathbf{S} can be identified to the principal directions and characteristic lengths of the disorientation distribution P (Equation 1), \mathbf{v}_i ($i \in \{1, 2, 3\}$) and θ_i , respectively.

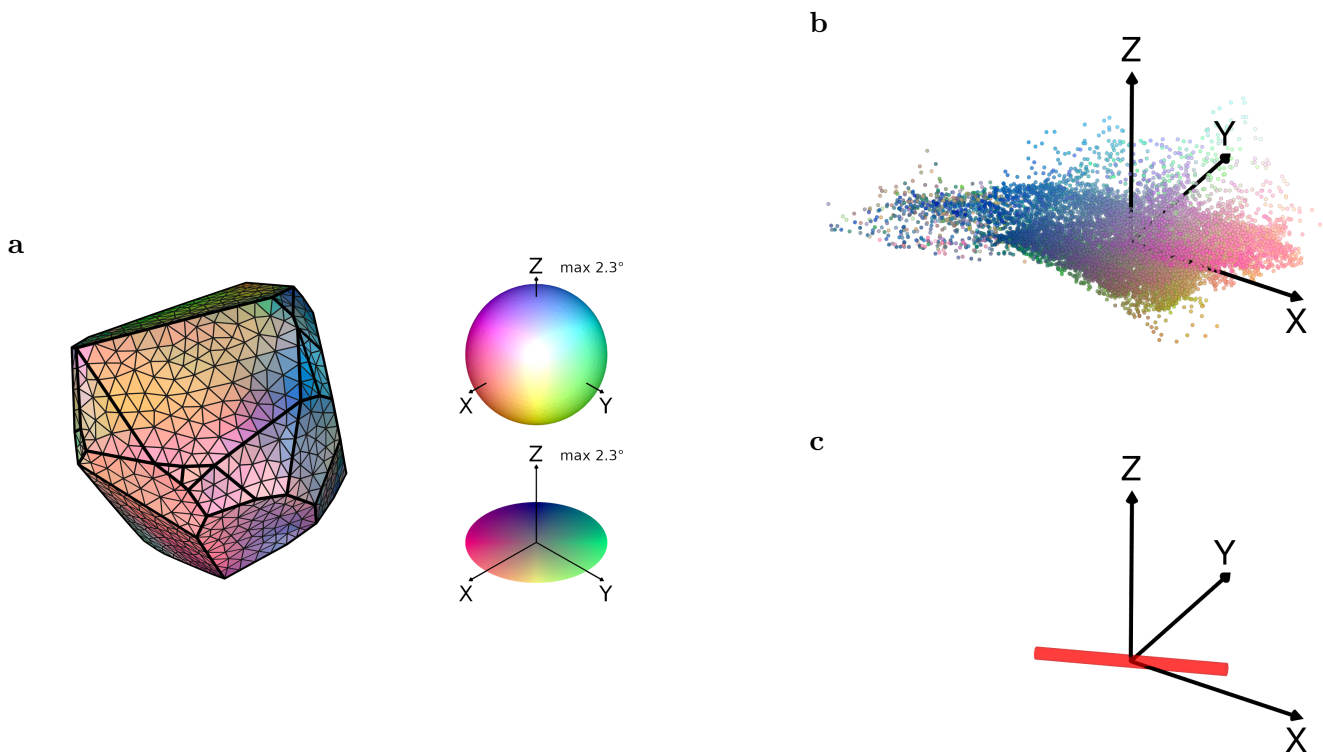


Figure 7: Illustration of the computation of the preferential disorientation axis from discrete orientation sets. Example of grain 1212 at $\varepsilon = 4.5\%$. (a) Disorientations (\mathbf{w}^α) represented on the mesh of the grain. The color key is defined in tangent space, as a ball of radius corresponding to a maximal disorientation of 2.3° . (b) Disorientations (\mathbf{w}^α) represented in tangent space, using the same colors as in (a). (c) Preferential disorientation axis (\mathbf{v}_1) computed from Equation 12.

⁵Fitting a 3-variate normal distribution to the discrete disorientation set of the grain, similar to the experimental approach, would be another possibility, but would lead to very close results for significantly larger complexity.

4 Results

Attributes of the intra-grain orientation distributions at successive strains were analysed for the same 466 grains in experiment and simulation. In the following, we first define some metrics to describe the orientation distributions and analyse trends in these metrics using distributions. We then look for grain-by-grain correlations between experiment and simulation, and correlations with the average grain orientation.

In the cases of results computed over all grains (average values, distributions, etc.), and due to the presence of (non-random) texture in the set of investigated grains (see Figure 1d), a texture correction is applied so as to obtain results that are representative of a texture-free material (in place of the polycrystal specifically considered). The texture correction defines a weight for each grain, from the size of the “local neighborhood” of its orientation (on the IPF, which is the appropriate space under the uniaxial symmetry condition). It follows that clustered orientations, which tend to over-represent particular orientations, have smaller weights, while isolated orientations, which represent large portion of possible orientations, have larger weights. The method is described in Section A, and the obtained (relative) grain weights vary from 0.07 to 8.

4.1 Average disorientation angle and anisotropy factor

The angular extent of the orientation distribution of a grain is typically quantified as the average disorientation angle with respect to the average orientation, $\bar{\theta}$ [4, 22], and is straightforward to compute in the case of discrete orientation sets (simulation results). In the case where only the anisotropy parameters of the orientation distribution (θ_i, \mathbf{v}_i) are known (experimental results), it can be computed with high accuracy as

$$\bar{\theta} = a (\theta_1^p + \theta_2^p + \theta_3^p)^{\frac{1}{p}}, \quad (13)$$

with $a = \sqrt{2/\pi}$ and $p = 1.58$ (see Appendix B). The distributions of the average disorientation angles at successive strains are provided in Figure 8, and the corresponding average values are provided in Table 3, for experiment and simulation. In both cases, the average disorientation angles increase gradually with strain. On average over all grains, the average disorientation angle increases almost linearly with strain, at rates of 0.08 and 0.18° per percent strain, for experiment and simulation, respectively. The constant rate of evolution can be explained by the fact that the deformation remains small enough so that the average orientation does not change significantly and the deformation conditions (slip rates, etc.) and therefore the reorientation conditions (including the disorientation distribution evolution) remain nearly the same [4]. The faster evolution in simulation was not observed in a previous work on the same material (deformed in hot plane strain compression to large strains) [4], but may be related to a smaller strain-rate sensitivity (m , see Equation 8), as using a larger value indeed reduces the θ_m values.

The strength of the anisotropy of the orientation distribution of a grain can be described by an “anisotropy factor”, θ_a , defined as

$$\theta_a = \theta_1 / \sqrt[3]{\theta_1 \theta_2 \theta_3}, \quad (14)$$

which takes a minimal value of 1 for an isotropic distribution. θ_a just serves for the comparison between experiment and simulation; specifically, it is not particularly related to any physical phenomenon, and other applications actually suggested expressions based on additive rather than multiplicative composition [3]. The distribution of the anisotropy factors are provided in Figure 9 for experiment and simulation, and the corresponding average values are provided in Table 3. Experiment and simulation show comparable distributions and average values of 1.7–2.0, while only the experimental anisotropy factors tend to increase with strain.

The experimental and simulated average disorientation angles and anisotropy factors at all strains are compared grain-by-grain in Figure 10. The θ_m values show appreciable correlation, with a linear correlation coefficient higher than 0.45 for strains of 1.5% and larger, while the anisotropy factors show only low correlation, if any.

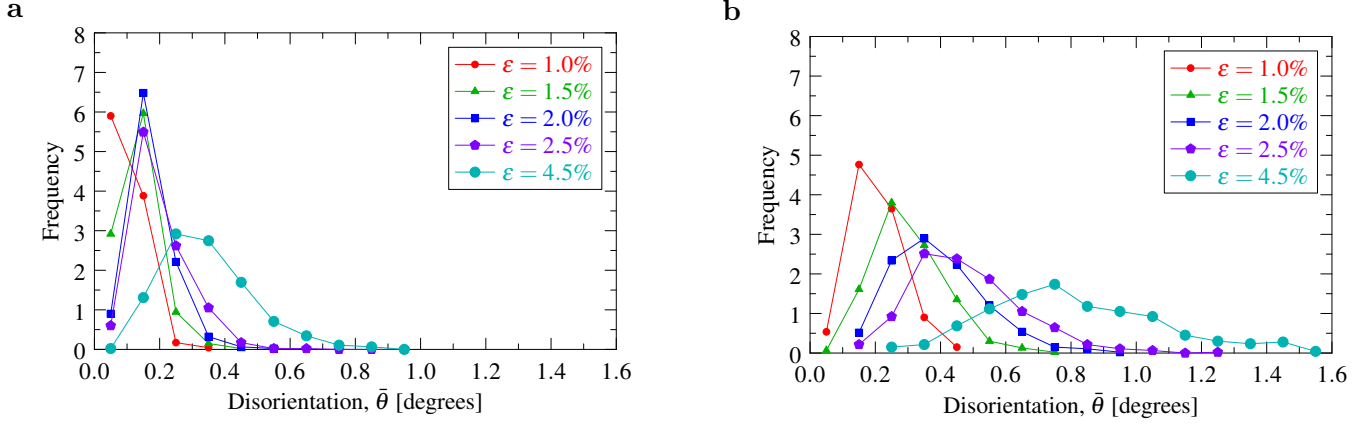


Figure 8: Distributions over all grains of the average disorientations, $\bar{\theta}$. (a) experiment and (b) simulation.

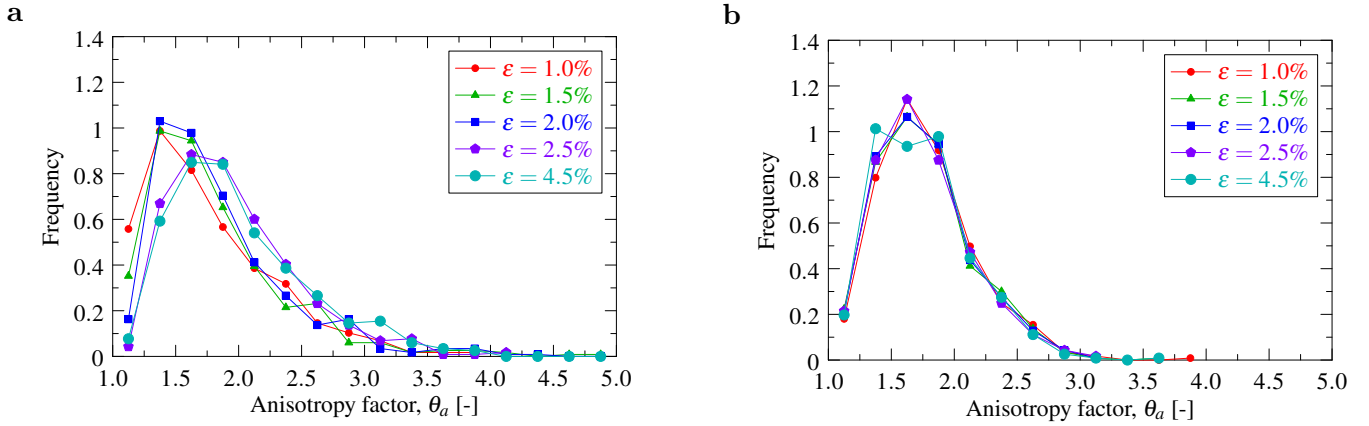


Figure 9: Distributions over all grains of the anisotropy factors, θ_a . (a) experiment and (b) simulation.

Strain	Average disorientation angle, $\bar{\theta}$ [°]		Average anisotropy factor, θ_a [-]	
	Experiment	Simulation	Experiment	Simulation
1.0%	0.10	0.20	1.75	1.78
1.5%	0.14	0.30	1.81	1.77
2.0%	0.17	0.39	1.85	1.76
2.5%	0.20	0.48	1.96	1.76
4.5%	0.35	0.82	2.03	1.75

Table 2: Evolution of the average disorientation angles and anisotropy factors with strain in the experiment and simulation.

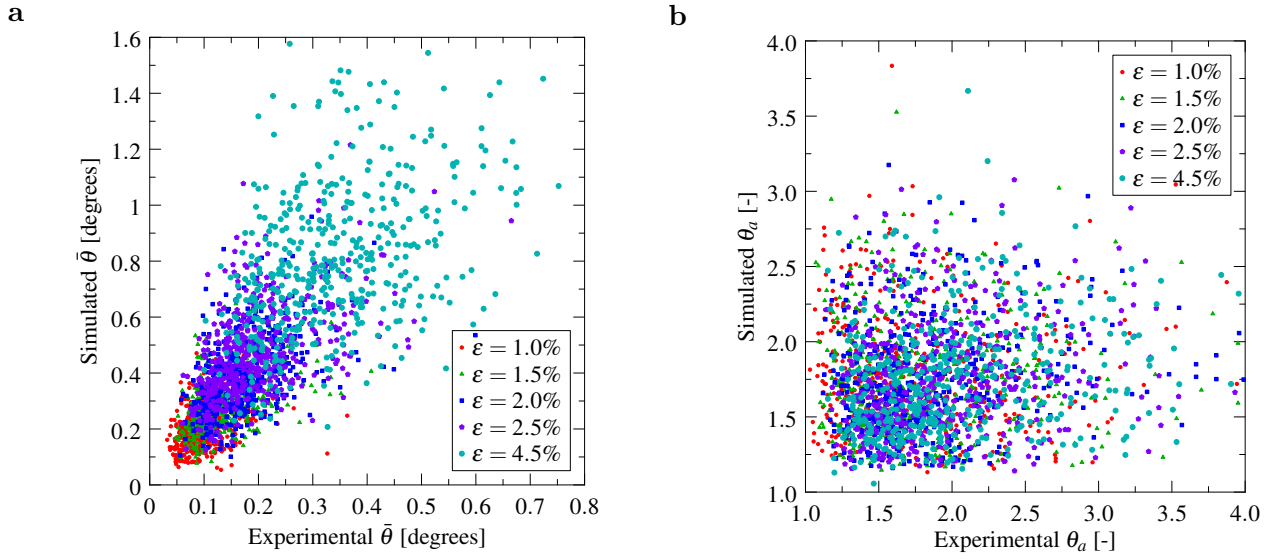


Figure 10: Grain-by-grain comparison between experiment and simulation of (a) the average disorientation angle ($\bar{\theta}$) and (b) the anisotropy factor (θ_a). Note the different x and y scales in (a).

Strain	Linear correlation coefficient [-]	
	Average disorientation angle, $\bar{\theta}$	Anisotropy factor, θ_a
1.0%	0.32	$\simeq 0$
1.5%	0.47	$\simeq 0$
2.0%	0.47	0.16
2.5%	0.48	0.17
4.5%	0.45	0.18

Table 3: Correlation between the grain average disorientation angles and anisotropy factors in experiment and simulation.

4.2 Preferential disorientation axis

The distributions of preferential disorientation axes (\mathbf{v}_1) at successive strains are provided in Figure 11, for both experiment and simulation. The equal-area projections are plotted onto the sample X–Y plane ($Z =$ tensile direction), with uniaxial symmetry applied to the density field. Figure 11 shows that, in the experiment, the axes are initially almost uniformly distributed and then become perpendicular to the tensile direction as strain increases. A smooth transition occurs with strain, and the distribution becomes clearly defined from a strain of 2%. In the simulation, the distributions are very similar at all strains and show the same distribution of axes perpendicular to the tensile direction. The simulated distribution is slightly more diffuse than the two final experimental ones (strains of 2.5 and 4%).

Figure 12 provides the distributions of the angles between the experimental and simulated preferential disorientation axes ($\mathbf{v}_1^{\text{exp}}$ and $\mathbf{v}_1^{\text{sim}}$, respectively) at successive strains. The distributions show that the agreement between experiment and simulation improves as strain increases, which is consistent with the progressive evolution of the experimental distributions toward the simulated distributions (distributions perpendicular to the tensile direction). A possible interpretation for an agreement improving with strain is that, at larger strains, and in particular after the elastic-plastic transition [44], the stress state “stabilizes” in a specific vertex of the yield surface, and that this occurs more rapidly in the simulation than in the experiment.

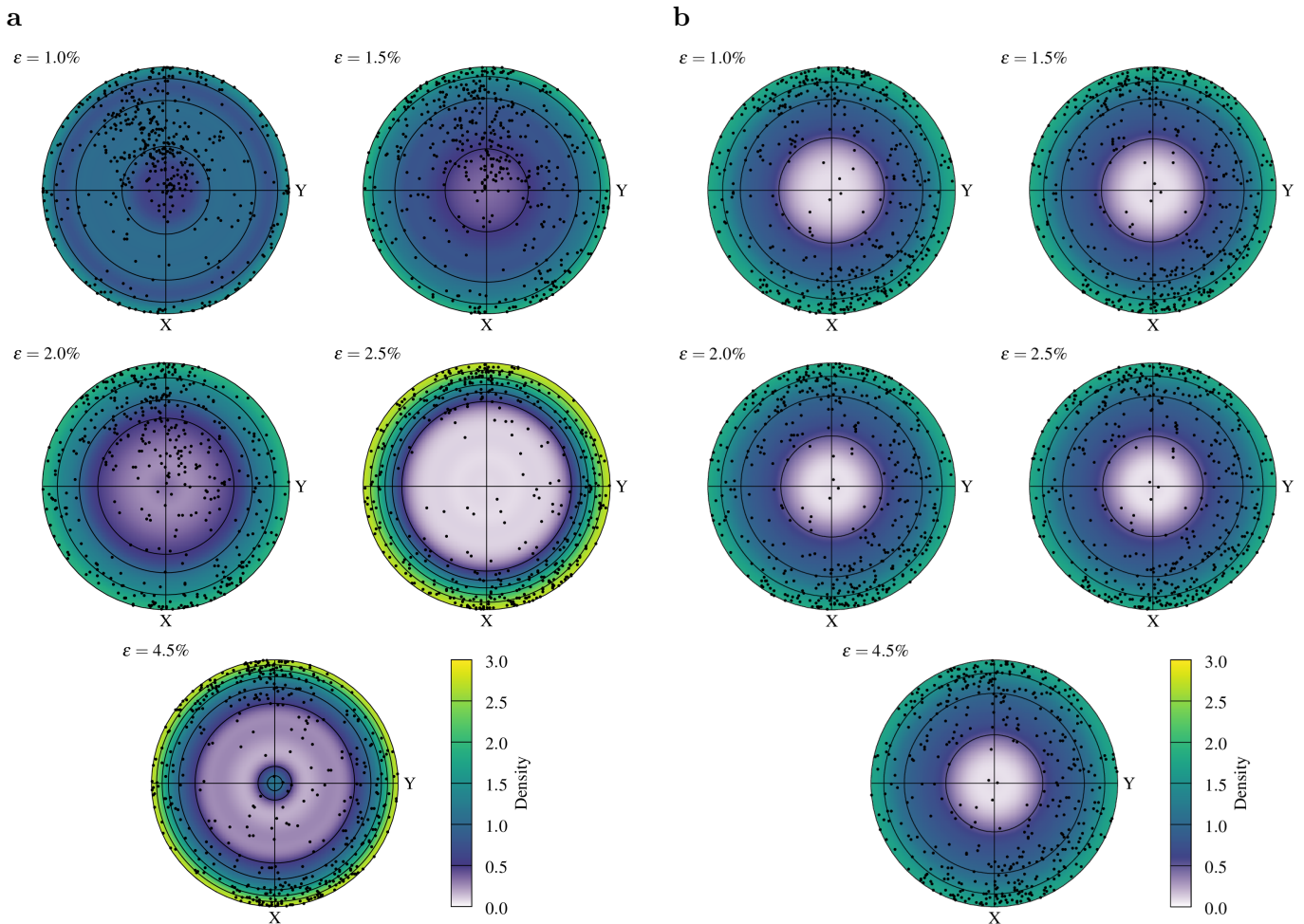


Figure 11: Distributions over all grains of the preferential disorientation axes, \mathbf{v}_1 , at increasing strains, in (a) experiment and (b) simulation. On the (equal-area) projections, the tensile axis (Z) is at the center of the figures, the data of each grain is represent by a dot, and uniaxial symmetry is applied to compute the density field (data averaging at constant distance from the origin).

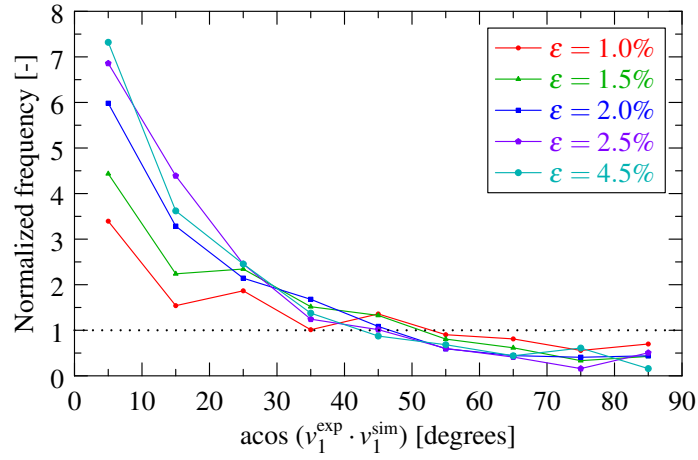


Figure 12: Distribution of the correlations between the experimental and simulated preferential disorientation axes ($\mathbf{v}_1^{\text{exp}}$ and $\mathbf{v}_1^{\text{sim}}$, respectively). The frequency plots are normalized with respect to the case of a random direction distribution (dotted line).

4.3 Correlation of the preferential disorientation axis with grain average orientation

To investigate the relationships between the preferential disorientation axes and the corresponding average orientations of the grains, the preferential axes can be plotted in the fundamental region of the Rodrigues orientation space [47]. The locations of the typical orientation fibers ($Z \parallel \langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$) are shown in Figure 13. The distributions of the preferential axes in the fundamental region, at successive strains and for both experiment and simulation, are plotted in Figures 14 and 15, as 3-D views and views along the tensile direction (Z), respectively. The views along Z somehow allow to “reduce” the data set according to the uniaxial symmetry condition. In Figure 14, the apparent non-uniform distribution of batons in Rodrigues space is due to the combined effects of the (non-random) texture and a higher density of Rodrigues space at the origin. A preferential disorientation axis is represented as a small baton as follows [4]:

- The radius and length are constant.
- The barycenter is on the average orientation.
- The axis is along the preferential disorientation axis, in orientation space.
- The color is related to the preferential disorientation axis components. Axes aligned with X , Y or Z are colored red, green or blue, respectively. Intermediate positions are represented by mixed colors, as indicated on Figures 14 and 15.

It can be clearly seen from the distributions that the experimental axes are of mixed directions at $\varepsilon = 1\%$, and that they rotate toward X - Y directions as strain accumulates, which is consistent with previous results (Figure 11). The simulated axes have similar X - Y directions at all deformations. In both experiment (at the largest strains) and simulation (at all strains), the preferential direction axes tend to be perpendicular to the tensile direction (Z) and to the X - Y component of the orientation vector. For example, orientations with a dominant X component (in Rodrigues space) have a preferential axis along Y , and, similarly, orientations with a dominant Y component (in Rodrigues space) have a preferential axis along X . This trend is global, and the regions about the $Z \parallel \langle 100 \rangle$, $Z \parallel \langle 110 \rangle$ and $Z \parallel \langle 111 \rangle$ fibers (shown on Figure 13) do not show any particularity.

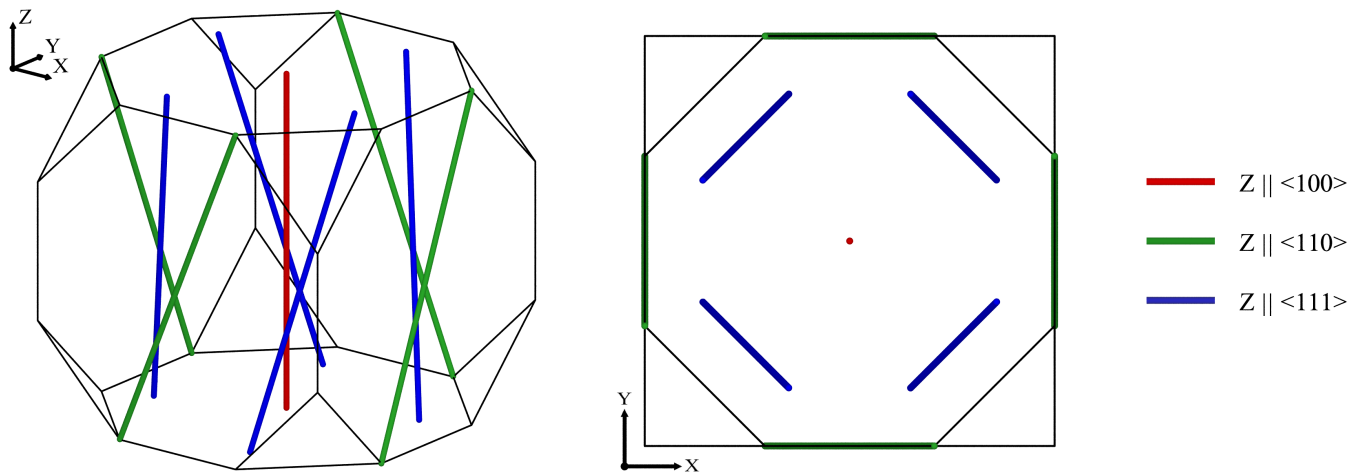


Figure 13: Ideal fibers for uniaxial tension (along Z) on an FCC polycrystal ($Z \parallel \langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$, which correspond to the three vertices of the standard triangle). Perspective and Z views.

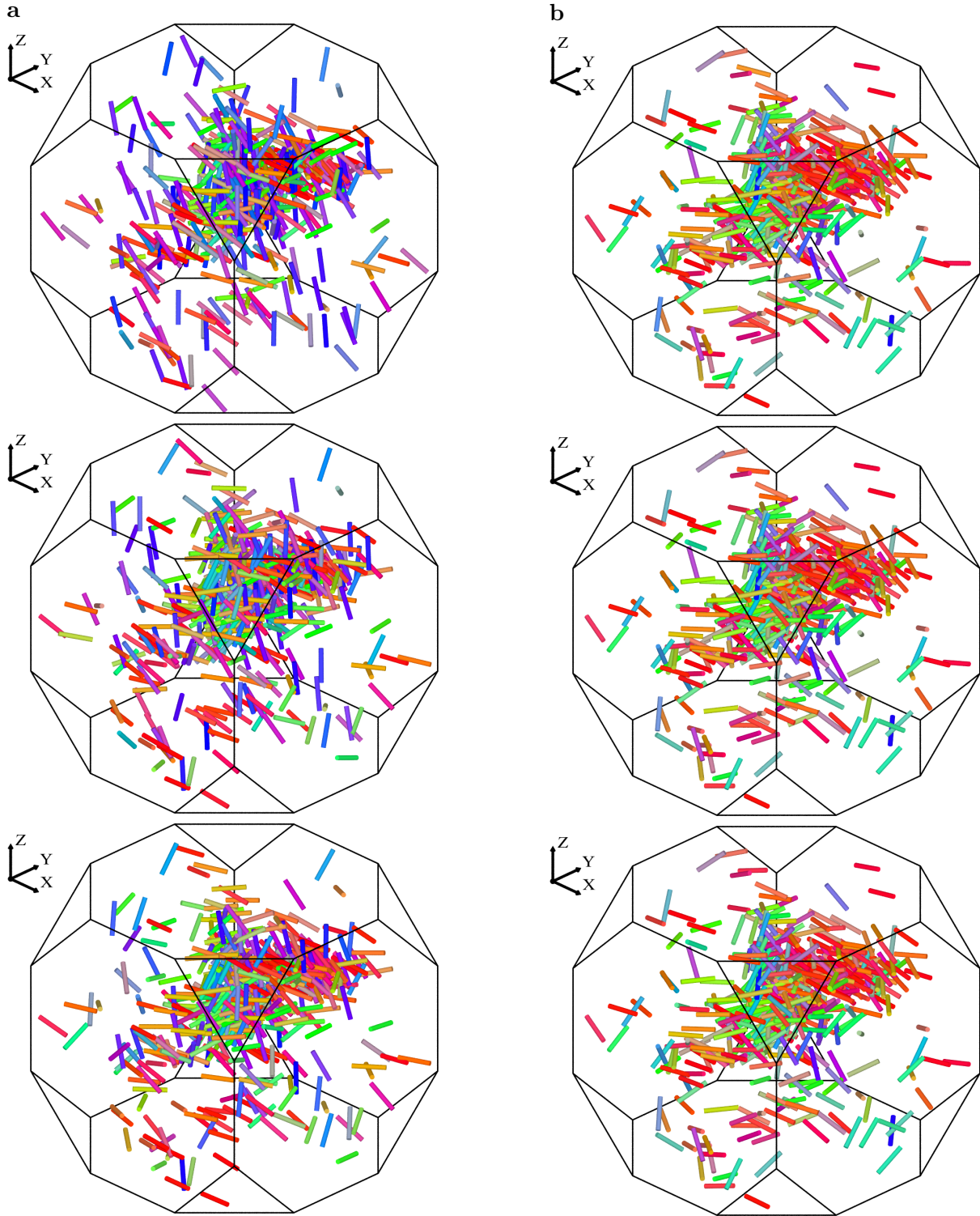


Figure 14: Correlation between the preferential disorientation axes and the average orientations of the grains, illustrated in the Rodrigues fundamental region (perspective view), for (a) experiment and (b) simulation. For each grain, the preferential disorientation axis is represented as a baton located at the average orientation of the grain. The color of the axis is related to its direction following the color key. From top to bottom, $\varepsilon = 1, 1.5, 2, 2.5$ and 4.5% , successively.

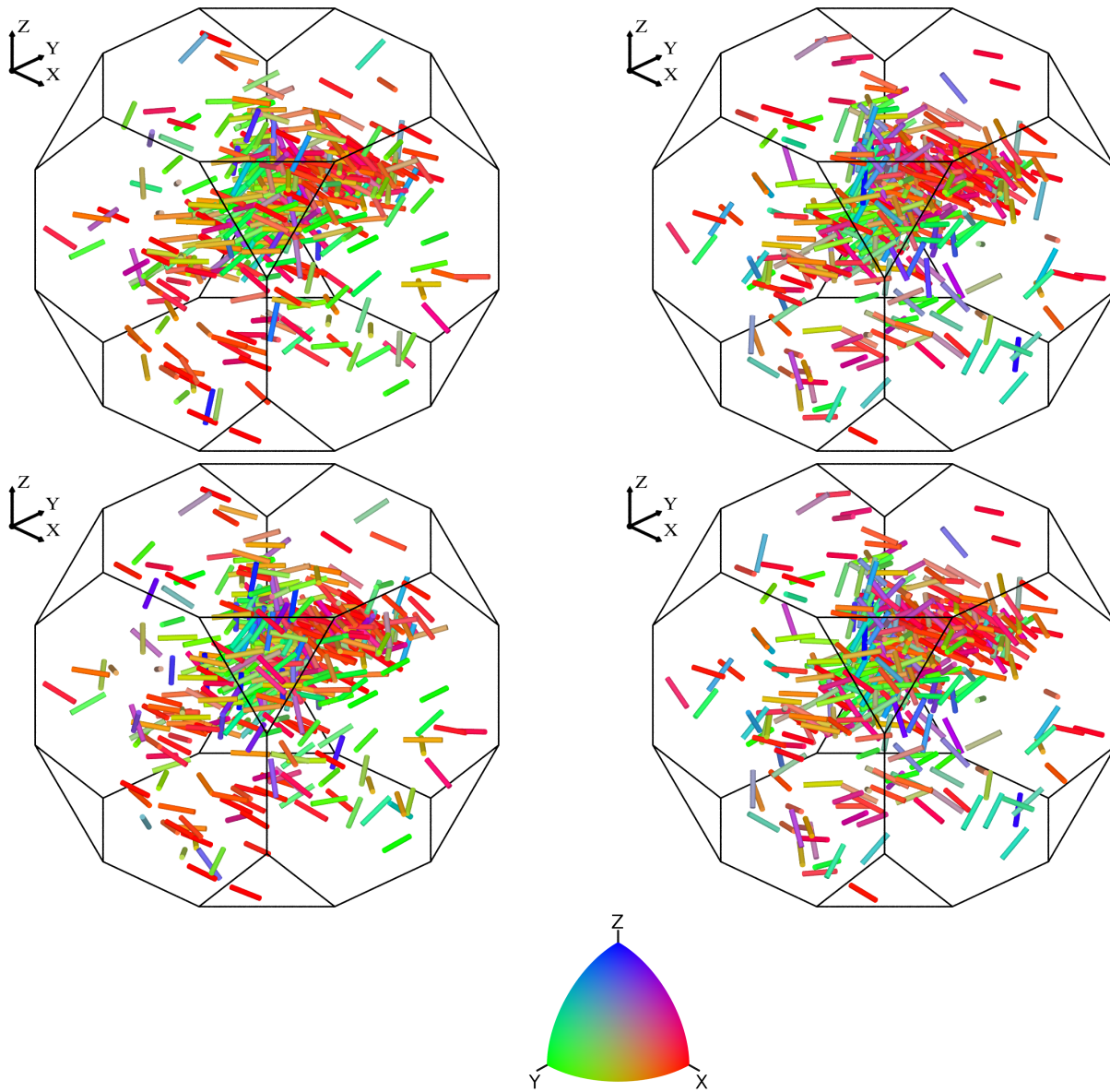


Figure 14: (continued)

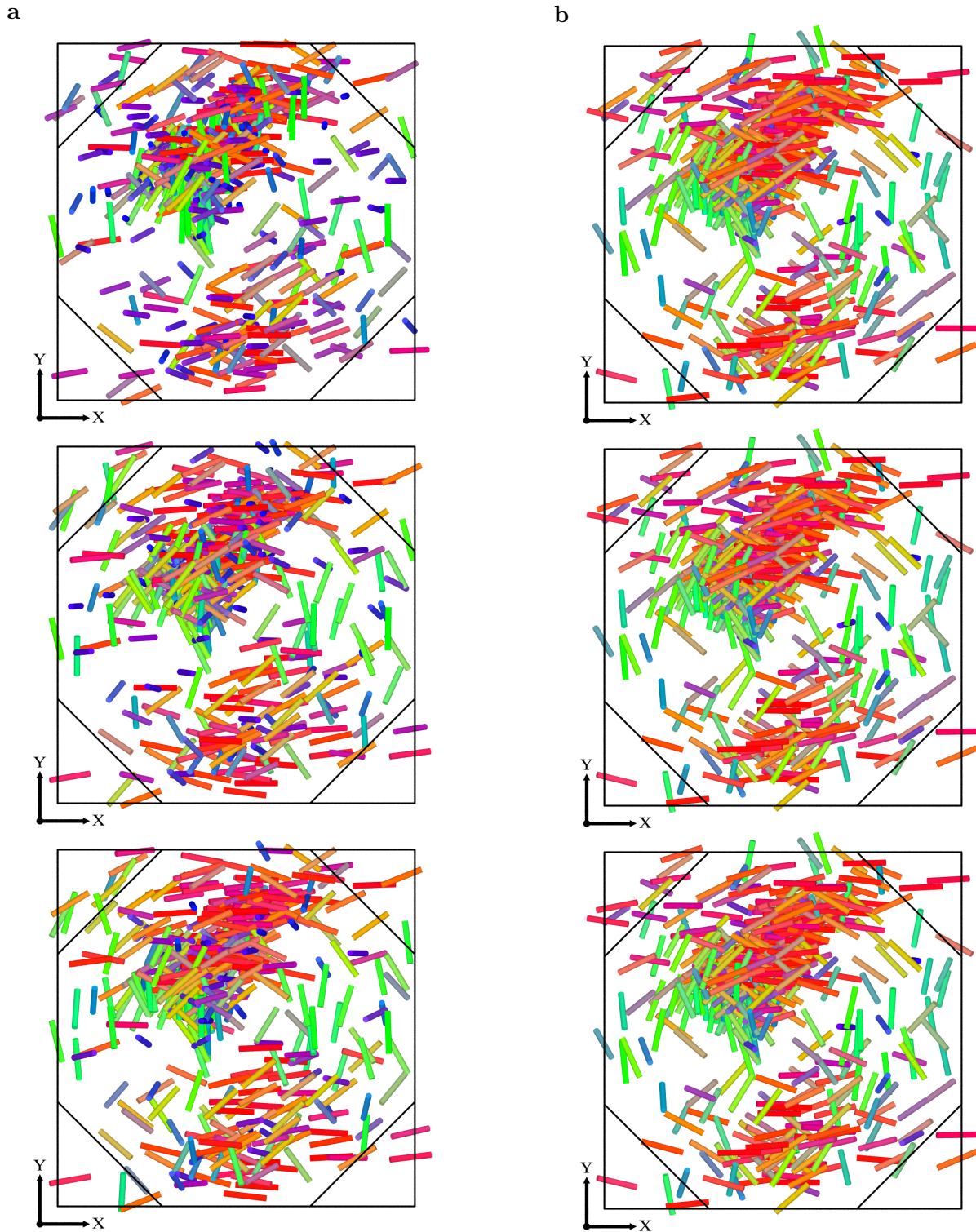


Figure 15: Correlation between the preferential disorientation axes and the average orientations of the grains, illustrated in the Rodrigues fundamental region (Z view), for (a) experiment and (b) simulation. For each grain, the preferential disorientation axis is represented as a baton located at the average orientation of the grain. The color of the axis is related to its direction following the color key. From top to bottom, $\varepsilon = 1, 1.5, 2, 2.5$ and 4.5% , successively.

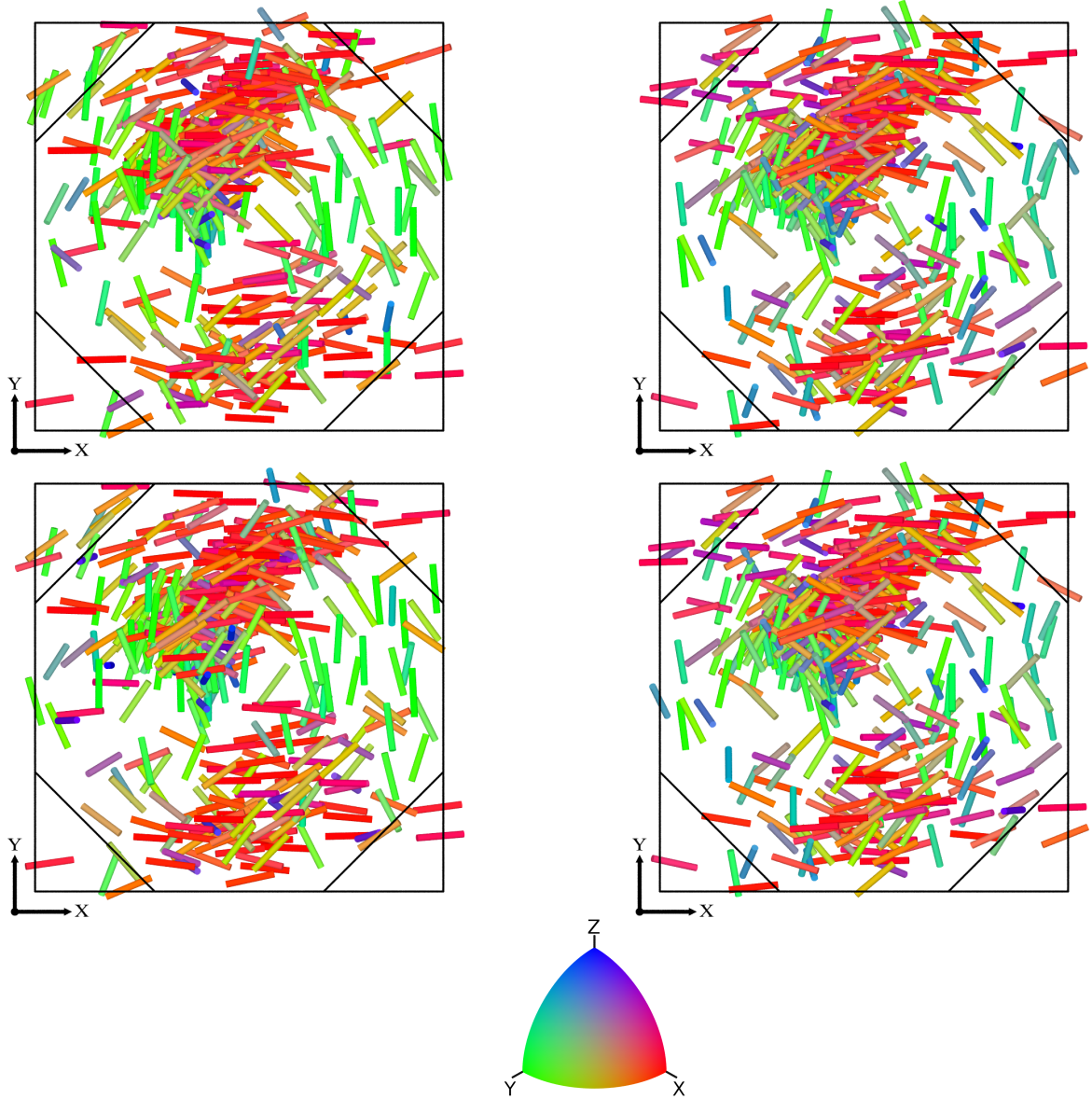


Figure 15: (continued)

5 Discussion

A set of 466 grains was used to analyse the evolution of the anisotropy properties of their orientation distributions, which can be considered as statistically significant [48]. Different metrics were used to describe the anisotropy properties of the orientation distributions, for which experiment and simulation show different degrees of agreement. Good experiment–simulation correlation was obtained on the average disorientation angles ($\bar{\theta}$, despite general overestimation by the simulation, Figures 8 and 10a) and on the preferential disorientation axes (\mathbf{v}_1 , Figures 11 and 12), which also showed similar orientation dependencies (Figures 14 and 15). In contrast, low (if any) correlation was obtained on the anisotropy factors (θ_a , Figures 9 and 10b).

Several conclusions can be drawn from these observations. First, the presence of a certain degree of agreement between experiment and simulation, which is of course essential to the study, constitutes a cross-validation of the two approaches and therefore a validation of the experiment-simulation approach as a whole. It confirms that, despite the approximations inherent in both approaches, the results are defined with sufficient precision to reveal some (and important) aspects of the material behavior. This supports the investigative philosophy adopted in this study, according to which global trends of the material behavior can be revealed without necessarily reproducing all the details involved. This is true both in the experiment, where the initial polycrystal structure and anisotropy properties of the orientation distributions are extracted only to certain precision, and in the simulation, where several assumptions or approximations are made, on the polycrystal structure, the slip law and the slip parameters (determined from the macroscopic stress-strain behavior). These approximations impact the results to different degrees and, together, are responsible for the discrepancies seen in the results. While an obvious way forward is to reduce them to improve both approaches and get a better agreement between them, which would need additional, detailed analyses, the areas of agreement in the current results also provide the important opportunity to build on them in order to improve our understanding of the material behavior. The simulation results are particularly helpful in this respect, as they include information that are not available in the experiment (or at least not as easily), such as the local stress⁶ and crystallographic slip rates.

Among all attributes of the orientation distributions, the preferential disorientation axis is of particular interest, as it provides the dominant direction of the orientation distribution, agrees well between experiment and simulation (including grain by grain) and shows quite clear dependency on orientation. Over all grains, the preferential disorientation axes distribute perpendicular to the tensile direction (Z) and perpendicular to the X–Y component of the orientation vector (in experiment, this develops progressively with strain). We also know from a previous work (done in hot plane strain compression) [4] that the preferential disorientation axis is closely related to the local deformation (especially the slip rates). In the following, in a similar approach, the simulation results are first used to relate the preferential disorientation axes to the slip geometry (Section 5.1). The simplified model presented in Ref. [4] is then used and extended to investigate the role of the average stress and intra-grain stress distribution on the preferential disorientation axis (Section 5.2).

5.1 Slip geometry and variability

In a grain, plastic deformation occurs by activation of slip on specific systems (among $\{111\}\langle 110\rangle$). Slip on a specific system generates lattice rotation about its spin vector, $\mathbf{t}^\alpha = \mathbf{m}^\alpha \times \mathbf{s}^\alpha$, where \mathbf{m}^α is the slip plane normal and \mathbf{s}^α is the slip direction. It follows that a variation of slip (about the average) on a system generates a variation of lattice rotations about its spin vector (\mathbf{t}^α), which finally leads to a 1-D orientation distribution along the spin vector (\mathbf{t}^α). The simultaneous activation of several systems generates lattice rotation variations about spin vectors of different directions, which finally leads to a general, 3-D orientation distribution. As the systems showing the larger slip variations produce the larger rotation variations, the 3-D

⁶While 3DXRD can in principle provide the average stress of a grain, this was not possible to do with sufficient relative precision for this material (which shows particularly low stresses) and this analysis. We will also look at the intra-grain stress distributions, which 3DXRD does not provide.

orientation distribution is anisotropic and preferentially elongated along the spin vectors of these systems. The orientation distribution of a grain therefore depends on the slip activity (and heterogeneity) inside the grain and holds a certain degree of information on it.

The slip activity inside the grains of the polycrystal can be investigated from the elemental slip rates. As the focus is on the distributions of orientations, the slip rates are also considered in terms of distribution (over all elements), with no consideration to their spatial locations within the grain. Values at the final strain ($\varepsilon = 4.5\%$) are considered, but considering other strains (or even the slips at final strain) would provide similar results, as the simulated preferential disorientation axes are largely independent of strain (see Figures 11b, 14b and 15b). To determine what are the characteristic directions (\mathbf{m}^α , \mathbf{s}^α and \mathbf{t}^α) of the most active slip systems, the characteristic directions of all systems are weighted by the corresponding average absolute slip rates, $|\dot{\gamma}^\alpha|$, and their distributions over all grains are analysed. For each grain, the average values of the characteristic directions, $\overline{\mathbf{m}^\alpha}$, $\overline{\mathbf{s}^\alpha}$ and $\overline{\mathbf{t}^\alpha}$, are used (12 values per grain). The distributions of $|\dot{\gamma}^\alpha| \overline{\mathbf{m}^\alpha}$, $|\dot{\gamma}^\alpha| \overline{\mathbf{s}^\alpha}$ and $|\dot{\gamma}^\alpha| \overline{\mathbf{t}^\alpha}$ over all grains are provided in Figure 16. Both the slip plane normals ($\overline{\mathbf{m}^\alpha}$) and slip directions ($\overline{\mathbf{s}^\alpha}$) are distributed at about 45° from the tensile direction (Z), and the spin vectors ($\overline{\mathbf{t}^\alpha}$) have X–Y directions, i.e. are perpendicular to the tensile direction (Z). These characteristics correspond to those of the systems of maximal Schmid factors for uniaxial tension.

The slip rate variability on a specific system of a grain is quantified as the standard deviation of the slip rates of all elements (considering, as before, the values at $\varepsilon = 4.5\%$). The slip rate variabilities are plotted against the (absolute) slip rates on Figure 17. It is clear that the systems of high slip rates exhibit that higher slip rate variability. The higher slip rate variabilities of the most active slip systems combined with their spin vectors being perpendicular to the tensile direction lead to the (experimental and simulated) preferential disorientation axis distributions perpendicular to the tensile direction (see Figure 11). The dependency of the variability of slip rate on the (absolute) average slip rate only applies to first order, however, as significant scatter also exists on Figure 17: systems of similar average slip rates may exhibit significantly different slip rate variabilities or, equivalently, similar slip rate variabilities can be observed for systems of different slip rates (this was also observed for higher strain rate sensitivity [4]). So, the (absolute) average slip rate and slip rate variability on a slip system also depend on the conditions that the system (and the grain) locally undergoes, especially in terms of the local stress and stress heterogeneity, which depends not only on the grain orientation but also on grain interaction.

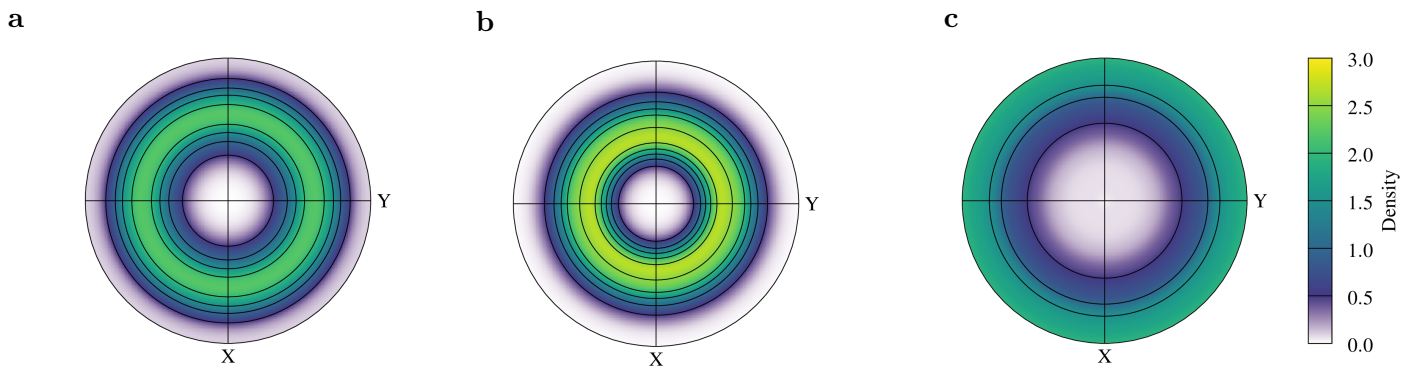


Figure 16: Geometry of the active slip systems for the 466 grains in simulation. Distributions of (a) $|\dot{\gamma}^\alpha| \overline{\mathbf{m}^\alpha}$, (b) $|\dot{\gamma}^\alpha| \overline{\mathbf{s}^\alpha}$ and (c) $|\dot{\gamma}^\alpha| \overline{\mathbf{t}^\alpha}$ in simulation (equal-area projections). Uniaxial symmetry is applied. For clarity, the discrete data (12 slip systems \times 466 grains) are omitted to show only their distributions.

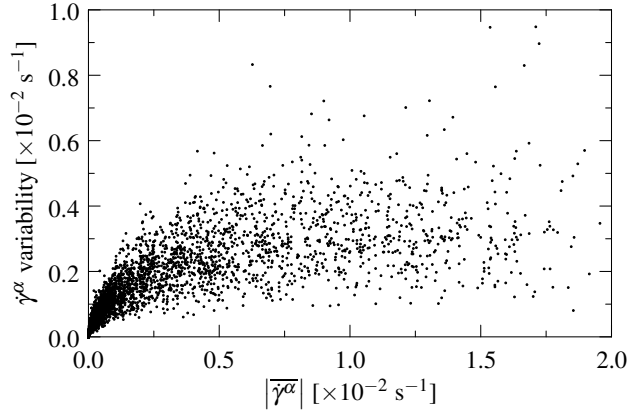


Figure 17: Relation between the slip rate variability and the average slip rate. The data are plotted for the 12 slip systems of each of the 466 grains in simulation.

5.2 Influence of the stress distribution

The lattice reorientation rate depends on the slip rates on the slip systems, which are themselves related to the resolved shear strengths (Equation 8) and, hence, to the stress. In the grains of a polycrystal, stress variation develops as a result of grain interaction. Under the assumption of zero local rigid-body rotation (or “spin”), the dependence of lattice reorientation on stress is given by

$$\frac{\partial \dot{\mathbf{r}}^*}{\partial \boldsymbol{\sigma}_v} = - \sum_{\alpha} \frac{\partial \dot{\gamma}^{\alpha}}{\partial \tau^{\alpha}} (\mathbf{t}^{\alpha} \otimes \mathbf{p}^{\alpha}), \quad (15)$$

where $\boldsymbol{\sigma}_v$ is the stress written in vector form [4]. The partial derivative is known from the kinetics expression given by Equation 8,

$$\frac{\partial \dot{\gamma}^{\alpha}}{\partial \tau^{\alpha}} = \frac{\dot{\gamma}_0}{m g^{\alpha}} \left| \frac{\tau^{\alpha}}{g^{\alpha}} \right|^{\frac{1}{m}-1}, \quad (16)$$

or, in terms of slip rate $\dot{\gamma}^{\alpha}$,

$$\frac{\partial \dot{\gamma}^{\alpha}}{\partial \tau^{\alpha}} = \frac{\dot{\gamma}_0}{m g^{\alpha}} \left| \frac{\dot{\gamma}^{\alpha}}{\dot{\gamma}_0} \right|^{1-m}. \quad (17)$$

For usual values of m in the range 0.02–0.15 (here 0.03), it is a strongly increasing function of τ^{α} and a nearly linear function of $\dot{\gamma}^{\alpha}$. The factor $(\mathbf{t}^{\alpha} \otimes \mathbf{p}^{\alpha})$, where \mathbf{t}^{α} is (as before) the spin vector, \mathbf{p}^{α} is the symmetrical Schmid tensor written in vector form and \otimes is the dyadic product between vectors, is fully geometrical and depends only on the crystal lattice orientation. Following Equations 15–17, the most active slip systems have a greater contribution to $\partial \dot{\mathbf{r}}^* / \partial \boldsymbol{\sigma}_v$, according to the $\partial \dot{\gamma}^{\alpha} / \partial \tau^{\alpha}$ factor.

By definition, $\partial \dot{\mathbf{r}}^* / \partial \boldsymbol{\sigma}_v$ provides the variation of the reorientation velocity vector as a function of a variation of the stress vector, and so the stress distribution inside a grain generates a reorientation distribution (and finally an orientation distribution) depending on $\partial \dot{\mathbf{r}}^* / \partial \boldsymbol{\sigma}_v$ (Equation 15). For future reference, $\partial \dot{\mathbf{r}}^* / \partial \boldsymbol{\sigma}_v$ can be subjected to a singular value decomposition,

$$\frac{\partial \dot{\mathbf{r}}^*}{\partial \boldsymbol{\sigma}_v} = \mathbf{U} \mathbf{S} \mathbf{V}^T, \quad (18)$$

where \mathbf{U} is a (3, 3) orthogonal tensor, \mathbf{S} is a (3, 6) diagonal tensor, and \mathbf{V} is a (6, 6) orthogonal tensor. The diagonal entries of \mathbf{S} are sorted in decreasing order. \mathbf{U} is a basis of the physical (real) space and \mathbf{V} is a basis of the stress space. It is important to note that the expression of $\partial \dot{\mathbf{r}}^* / \partial \boldsymbol{\sigma}_v$ (Equation 15) was obtained under only the assumption of zero rigid-body rotation (spin) and therefore holds a general character. It is to be computed for a nominal stress (typically the average stress), while the reorientation distribution is obtained

from the stress distribution about the nominal stress. However, different models can be used to determine the nominal stress, and different assumptions can be made on the stress distributions to compute the resulting reorientation distributions.

In Ref. [4], a Taylor (iso-strain) assumption was used, and a random, isotropic stress distribution (random vectors in stress space) was then considered. The Taylor model is well-known for providing good first-order predictions of the grain rotations and textures [26,49], while an isotropic stress distribution is a natural first-approach distribution, advantageously leads to a reorientation velocity distribution of principal directions simply given by the rows of \mathbf{U} and magnitudes given by the associated diagonal entries of \mathbf{S} , and has proven effective in Ref. [4]. It is interesting to start with this simple configuration to determine how well it can reproduce the observed disorientation distributions (and in particular the preferential disorientation axes) and so get a first idea of how much they depend on the nominal stress and stress distribution. Note that, using these assumptions, the resulting distribution will necessarily show greater orientation dependency than the experimental or simulated ones, as the preferential disorientation axes depend only on orientation. The distribution of the preferential disorientation axes resulting from these assumptions is provided in Figure 18. It can be seen that the equal-area projection is in good agreement with the experimental and simulated ones (see e.g. Figure 11a,b at $\varepsilon = 4.5\%$), but that the distribution in orientation space (Figure 18b versus Figures 14 and 15) shows less agreement (while good agreement was obtained for hot plane strain compression [4]). So, considering an idealized configuration consisting of a Taylor stress and an isotropic stress distribution does not reproduce the distribution of the preferential disorientation axes in a region surrounding the $Z \parallel \langle 100 \rangle$ fiber where the axes are oriented parallel (rather than perpendicular) to the X–Y component of the orientation vector.

Given that the idealized configuration does not fully reproduce the observed (experimental or simulated) orientation dependency of the preferential disorientation axes, the following question arises: what is (or are) the driving factor(s) for the difference (especially around $Z \parallel \langle 100 \rangle$), in terms of the assumptions made in the idealized configuration? As per the specificities of the idealized configuration, the two main factors may be: (1) the assumption of iso-strain (Taylor model) to compute the nominal stress and $\partial \dot{\mathbf{r}}^* / \partial \sigma_v$, and (2) the assumption of an isotropic stress distribution to compute the preferential disorientation axes. Another possible factor is (3) the assumption of zero (or negligible) local rigid-body rotation, which, based on the analysis made in Section 5.1, should not play an important role, but is also considered in the following for completeness.

The procedure to determine the relative influences of the three main assumptions is to consider the idealized configuration and relax each assumption independently, as follows:

1. Relaxed iso-strain assumption: the finite-element average stress is considered in place of the Taylor stress. This provides a new value of $\partial \dot{\mathbf{r}}^* / \partial \sigma_v$, from which the preferential disorientation axis of the grain is computed as previously, by singular value decomposition (Equation 18).
2. Relaxed isotropic-stress-distribution assumption: the (discrete, anisotropic) finite-element stress distribution is considered instead of the isotropic distribution. So, the nominal value of $\partial \dot{\mathbf{r}}^* / \partial \sigma_v$ is still used, but the finite-element stress vectors (with respect to the average stress) are then multiplied by $\partial \dot{\mathbf{r}}^* / \partial \sigma_v$ to obtain the corresponding (discrete) reorientation rate distribution, from which the preferential disorientation axis is computed as for the simulation results, using Equation 12.
3. Relaxed zero-spin assumption: the (discrete, anisotropic) finite-element spin rate distribution is introduced. The finite-element spin rate vectors (with respect to the average spin) are combined with the reorientation rate vectors resulting from the isotropic stress distribution as per the standard composition [4] to obtain a new reorientation rate distribution, whose anisotropy properties are computed as in the simulation, using Equation 12 (due to the discrete nature of the spin rates, the isotropic stress distribution is also considered as discrete, as in configuration 2).

Figure 19 provides the preferential disorientation axes obtained in the three configurations, as equal-area projections and distributions in orientation space (to be compared to Figures 11, 14 and 15 at $\varepsilon = 4.5\%$). In addition, the correlation to the experimental disorientation axes ($\boldsymbol{v}_1^{\text{exp}}$) is quantified as the average value of the angles between the experimental and predicted axes (same metric as in Figure 12). The value for the finite element simulation is 37° , which is the value to ultimately reproduce by the idealized and relaxed configurations. The obtained values are 46° for the idealized configuration (iso-strain and isotropic stress distribution), and 38° , 56° and 47° for the three successive relaxed configurations. It is clear from these results that considering the finite-element average stresses instead of the Taylor stresses (configuration 1) largely corrects the preferential disorientation axes in the $Z \parallel \langle 100 \rangle$ region, and gives a degree of agreement very close to the experiment–simulation one. Conversely, considering an anisotropic stress distribution or a non-zero spin distribution (alone) does not improve the distribution. This can be explained by several reasons. First, good results with an isotropic stress distribution (configuration 1) indicate that the preferential disorientation axes are controlled by the shape of $\partial \dot{\boldsymbol{r}}^* / \partial \sigma_v$ rather than by the shape of the stress distribution. $\partial \dot{\boldsymbol{r}}^* / \partial \sigma_v$ depends on the crystal orientation, (non-linearity of the) slip law, and average stress of the grain, which ensures proper selection of the active slip systems. Second, the lack of improvement when considering the actual stress distribution (variations about the average) can be related to the fact that it is not considered about the correct nominal stress. Finally, the spin, as not being intrinsically associated to particular spatial directions (unlike slip), does not involve a particular distribution of the associated reorientation directions. A last natural choice is to combine configurations 1 and 2, which leads to a value of 39° , similar to the one obtained with configuration 1 alone, thereby confirming that the average stress is the main driving factor.

6 Conclusions

The orientation distributions developing within individual grains of an aluminium polycrystal deformed in tension were experimentally characterized by far-field 3D X-ray diffraction microscopy and simulated using the finite-element method. A statistically significant set of 466 grains was considered. In the experiment, a method was presented to unambiguously determine the anisotropy properties of the orientation distributions from the broadening of the diffraction spots. In the simulation, each grain was discretized into several hundreds of elements, also giving access to intra-grain orientation distributions. The anisotropy properties of the orientation distributions were analysed in terms of angular extent (average disorientation angle, $\bar{\theta}$), anisotropy factor (θ_a) and preferential disorientation axis (\boldsymbol{v}_1). A high degree of variability of the results was found among grains both in experiment and simulation. The average disorientation angles were found to increase almost linearly with strain and to be in appreciable agreement between experiment and simulation, although evolving faster in simulation. The anisotropy intensity was found to remain similar during deformation, with typical values in the range 1.5–3, with only a slow increase with strain in experiment. The preferential disorientation axes were found to be mainly oriented perpendicular to the tensile direction (Z) and perpendicular to the X–Y component of the Rodrigues orientation vector. Here, experiment and simulation are in good agreement. An analysis based on the simulation results revealed that the development of preferential disorientation axes can be explained by larger slip variations developing on the most active slip systems. Using a simplified model, it was possible to show that an accurate estimate of the local (average) stress is essential to properly predict the preferential disorientation axis, especially for orientations about the $Z \parallel \langle 100 \rangle$ fiber, which is properly done by the finite-element simulation. The intra-grain stress distribution (about the average) has comparatively less influence and can be assumed as isotropic to first order.

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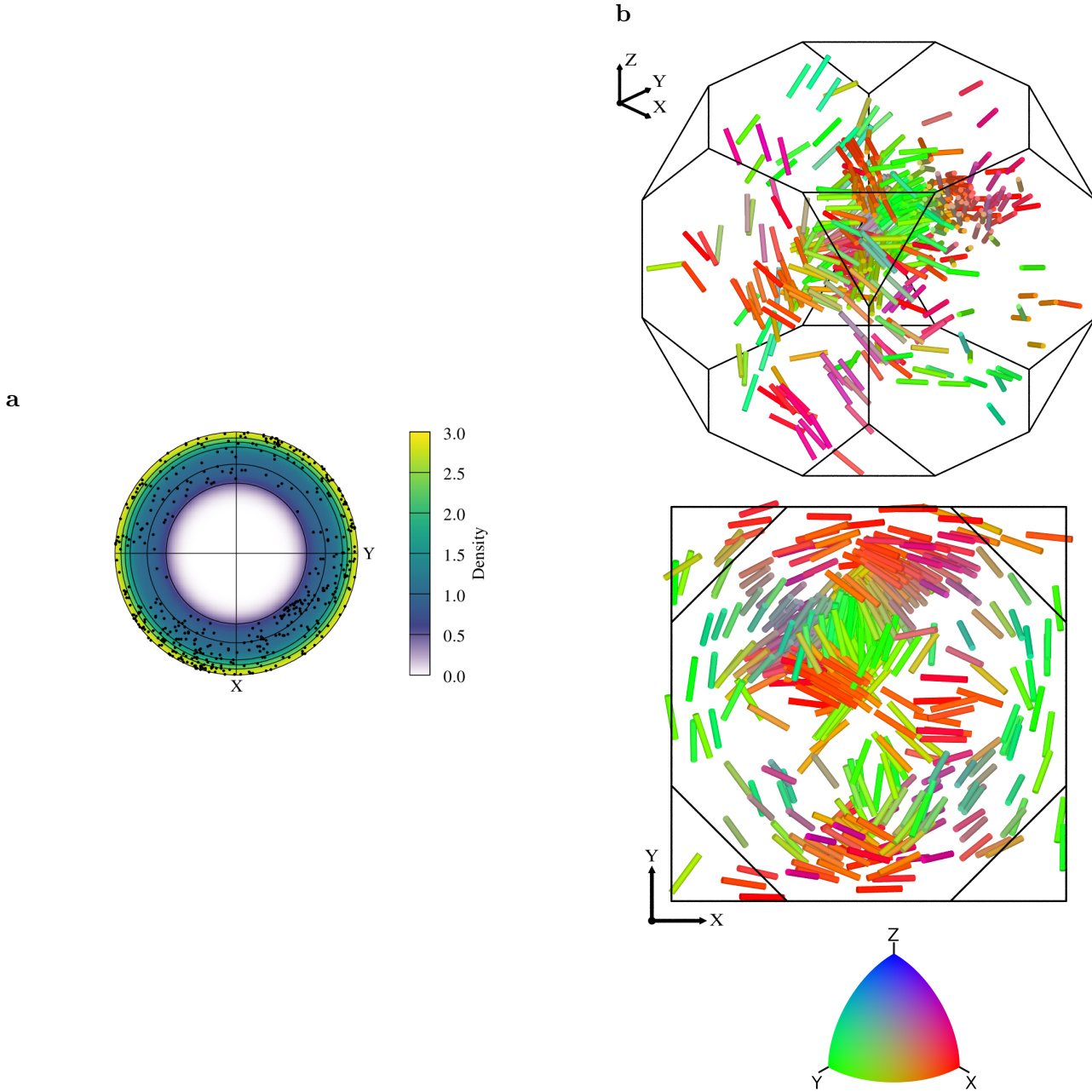


Figure 18: Preferential disorientation axes resulting from an isotropic stress variability shown as (a) distribution over all orientations (equal-area projections) and (b) correlation with the associated average orientations.

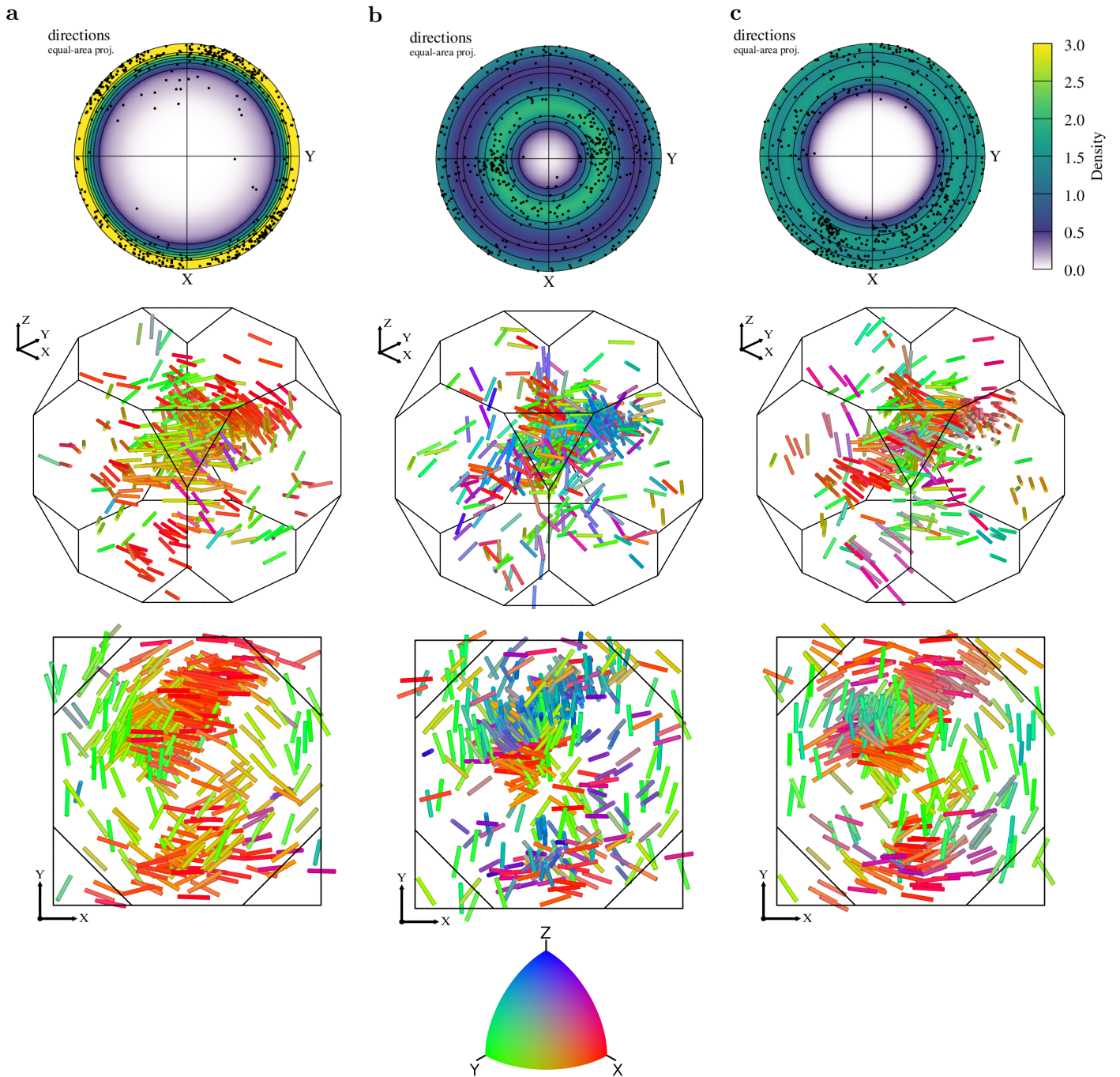


Figure 19: Preferential disorientation axes resulting from the idealized configuration and (a) the relaxed iso-strain assumption, (b) the relaxed isotropic-stress-distribution assumption and (c) the relaxed zero-spin assumption.

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A Orientation weights and texture correction

In the presence of a preferential grain orientation distribution (or (non-random) “texture”) in the investigated polycrystal, weights can be defined from the grain orientations and used when computing results over all grains, so that the obtained results are representative of a general, texture-free material. This process is referred to as “texture correction”.

Under uniaxial sample symmetry, orientations can be plotted on the standard triangle (inverse pole figure), where each orientation is represented by a unique point corresponding to the position of the tensile axis in the crystal coordinate system. For each orientation, a weight can then be defined from the fraction of all possible orientations (all positions of the standard triangle) the orientation represents. This is done by Voronoi tessellation, by which each orientation generates a cell that corresponds to the region that is closer to the orientation than to any other orientation. The weight of an orientation is then defined as the (relative) surface area of its associated Voronoi cell. (Equal-area projection is considered for the inverse pole figure, so that the surface areas of the orientation cells are not biased by the projection itself.) The more orientation are “clustered”, the smaller their weights; conversely, the more “isolated” an orientation is, the larger its weight. For a texture-free material, all orientations have (roughly) equal surface areas.

The resulting tessellation is provided in Figure 20a, and the (normalized) surface areas of the orientations vary from 0.07 to 8, while 90% range from 0.2–2.5. As expected, smaller (normalized) surface areas are obtained for orientations where the ODF is larger (compare Figures 20a and 1d). The present definition of orientation weights is therefore similar (still generally non-equivalent) to considering the inverse values of the ODF.

B Computation of the average disorientation angle

For n -D isotropic, normal disorientation distributions, the expression of the average disorientation angle ($\bar{\theta}$) as a function of the standard deviation of the normal distribution in one direction (n), is given by [6]

$$\bar{\theta} \simeq C(n) \sigma, \quad (19)$$

where

$$C(n) = \sqrt{2} \frac{\Gamma[(n+1)/2]}{\Gamma(n/2)}, \quad (20)$$

which yields

$$C(1) = \sqrt{2/\pi} < C(2) = \sqrt{\pi/2} < C(3) = 2\sqrt{2/\pi}. \quad (21)$$

For a 3-D anisotropic disorientation distribution, the expression of the average disorientation angle ($\bar{\theta}$) must involve the standard deviations of the normal distributions in the three principal directions (θ_1 , θ_2 and θ_3). The scaling factors of n -D isotropic distributions given in Equation 21 ($C(\bullet)$) also applies to the special cases of 3-D anisotropic distributions of standard deviations (*i*) $\theta_1 = \sigma$, $\theta_{2,3} = 0$ (for $C(1)$), (*ii*) $\theta_{1,2} = \sigma$, $\theta_3 = 0$ (for $C(2)$) and (*iii*) $\theta_{1,2,3} = \sigma$ (for $C(3)$) and can be considered as reference values to be reproduced (or closely approximated) by any expression of $\bar{\theta}$ generalized to the anisotropic case. We propose an expression proportional to the L^p -norm of the (θ_1 , θ_2 , θ_3) vector:

$$\bar{\theta} = a (\theta_1^p + \theta_2^p + \theta_3^p)^{\frac{1}{p}}. \quad (22)$$

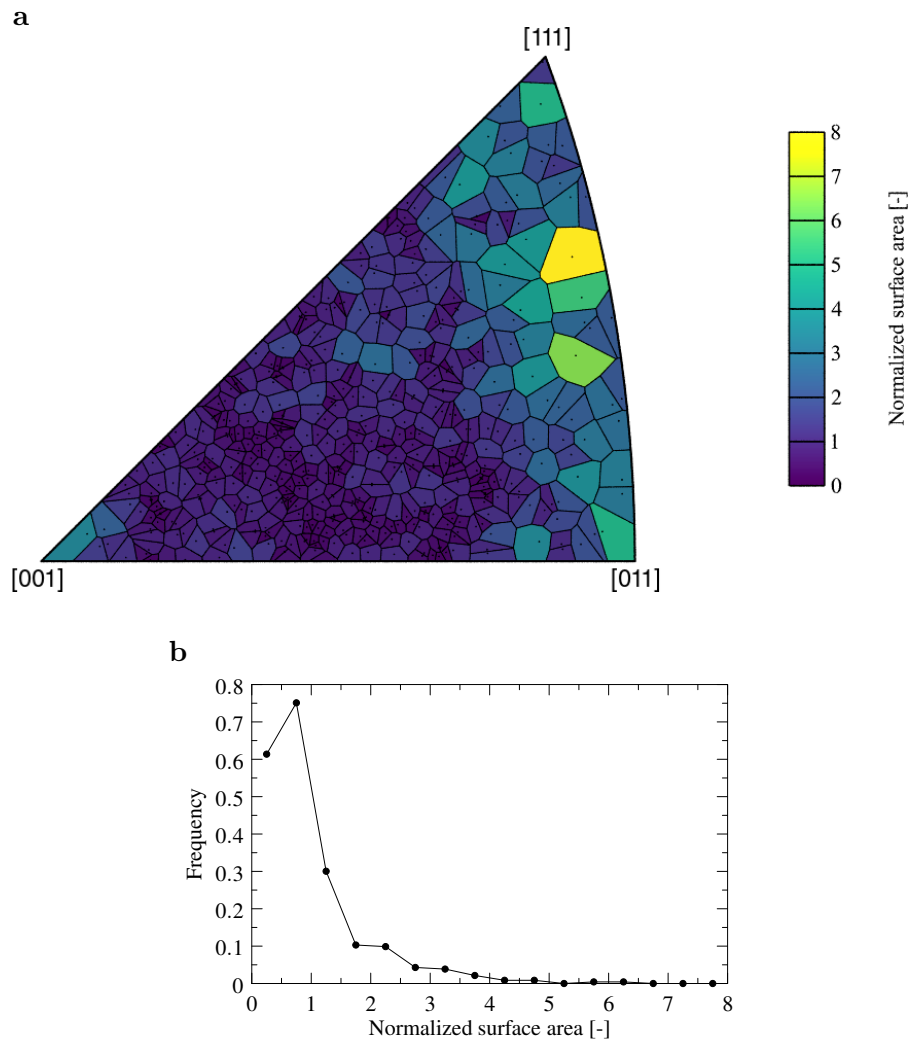


Figure 20: Computation of orientation weights via Voronoi tessellation on the standard triangle (inverse pole figure) under equal-area projection. (a) Voronoi tessellation, where the orientations are represented by the black dots and the Voronoi cells are colored according to their (normalized) surface areas. (b) Distributions of the orientation weights over all grains.

The values of a and p can be determined by comparing the $\bar{\theta}$ values provided by Equations 19 and 22 for different values of n (to first order, and knowing that the problem is overdetermined). Considering $n = 1$, we get $a = C(1) = \sqrt{2/\pi}$. Then, following simple mathematical manipulations, $n = 2$ yields $p = \ln(2)/\ln(\pi/2) \simeq 1.535$ while $n = 3$ yields $p = \ln(3)/\ln(2) \simeq 1.585$. The similar values of p obtained for $n = 2$ and $n = 3$ (both of which would also apply to $n = 1$), which correspond to extremal values of θ_i (in their respective domains of definition), show that the expression of $\bar{\theta}$ provided by Equation 22 can be appropriately used. An “optimal” value of p can be obtained by fitting Equation 22 to data obtained from numerical experiments. To do so, θ_2 and θ_3 were varied over their respective domains of definition ($\theta_2 \in [0, \theta_1]$ and $\theta_3 \in [0, \theta_2]$), and, for each value, 10^6 data points were generated following the corresponding 3-variate normal distribution, and the actual value of $\bar{\theta}$ was computed. The data are shown on Figure 21, and the identification provided $p = 1.58$. It is clear from Figure 21 that Equation 22 with $a = \sqrt{2/\pi}$ and $p = 1.58$ closely approximates the numerical values. The average error is 0.32% and the maximum error is 1.2%.

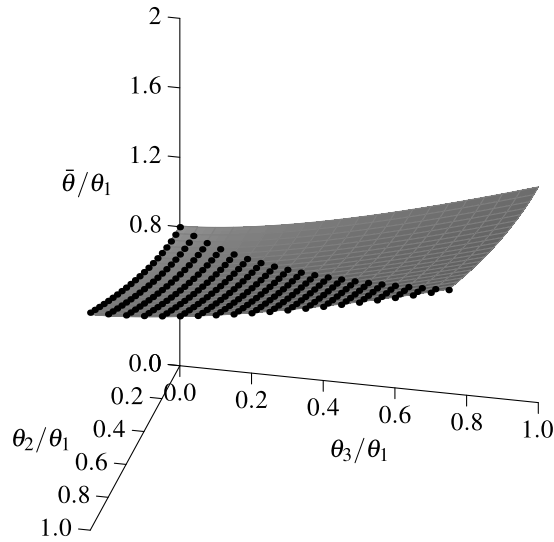


Figure 21: Relation between the average disorientation angle ($\bar{\theta}$) and the standard deviations about the principal disorientation axes (θ_1 , θ_2 and θ_3). The dots represent the numerical values, and the surface represents the analytical approximation.

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