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On the statistical significance of grain-scale lattice rotation results

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Abstract

The statistical significance of grain-scale lattice rotation results is analysed. The case of the results of Ref. [1] is specifically considered. Quantitative elements of the theory of statistics are applied to determine precisions (standard errors) of the results and the size of the representative volume element (RVE), in terms of the minimal number of grains necessary to obtain the results. It is shown that the results of Ref. [1] are defined to sufficient precision to support the conclusions made. In general, the RVE size, i.e. the numbers of grains necessary to derive conclusions on the rotation trends over all grains, range between a few tens and about 200. The proposed method is general and can easily be applied to other data sets to determine their own precisions and RVE sizes.

1 Introduction

Grain-scale experimental observations of lattice rotations are essential to develop a better understanding of plastic deformation of polycrystalline materials and its impact on their microstructure evolutions, and to validate crystal plasticity models. Several methods have been used, e.g. based on electron backscatter diffraction (EBSD, in some cases associated to the use of a "split sample", by which grains are followed on an internal surface of a sample) [1–4], or synchrotron X-ray diffraction [5–8]. As using these methods and analysing the associated results is generally long and tedious, limited numbers of grains are usually considered: 58 in Ref. [2], 45 in Ref. [3], 95 in Refs. [5, 9], about 200 in Ref. [4], 175 in Ref. [1], about 150 in Ref. [6], 172 in Ref. [7] and 466 in Ref. [8] (somewhat of an exception). In these works, aluminium alloys were generally used [1–5, 7–9], and the samples were subjected to plane strain compression (or rolling) [1–4] or tensile deformation [5–9].

While a number of grains in the range 50–200 seems sufficient for most studies (depending on the results of interest), the issue of the statistical significance was generally not discussed, and, in Ref. [10], Pirgazi and Kestens specifically questioned the experiment and results reported in Ref. [1] and a related article [11] (for which data were made openly available [1, 12]) due to their "*poor statistical relevance*": "*Using the Taylor model and after tracking the individual orientations during hot deformation of an aluminum split-sample, Quey et al. [1] and Panchanadeeswaran et al. [2] compared the modelled orientation rotations with the experimental results. Despite their similar experiments, they ended up with totally different conclusions regarding the precision of the Taylor model in prediction of crystallographic orientations after deformation. One possible explanation for the disagreement between their conclusions can be the poor statistical relevance of their experiments; Quey et al. [1] and Panchanadeeswaran et al. [2] tracked the total number of 157 and 58 grains during deformation, respectively. A more precise investigation with a larger number of grains is therefore needed to derive a solid conclusion.*". However, the authors did not substantiate their assertions, nor did they provide a statistical analysis of their own experimental results. Results of greater statistical significance do not necessarily invalidate previous works, especially when they do not report on the same type of results, or when the previous works concern different (or broader) conditions.

In this article, the general issue of the statistical significance of grain-scale lattice rotation results is systematically and quantitatively addressed by specifically analysing the main results reported in Ref. [1] (later simply referred to as "experimental results") and Ref. [11] (comparison to simulation).

2 Theoretical basis

The general concept of "statistical significance" can be approached quantitatively based on the theory of statistics [13]. Given a set of n uncorrelated values of standard deviation σ, the standard error of the average value, σ_m, is given by

$$\sigma_m = \frac{\sigma}{\sqrt{n}}, \tag{1}$$

independent of the type of distribution of the values (normal distribution or not). It is then common practice to consider a precision on the average equal to $\pm 2\,\sigma_m$, which provides 95% confidence, while a precision equal to $\pm 3\,\sigma_m$ provides 99.7% confidence. These confidence intervals correspond to those of a normal distribution. Indeed, average values computed from different samples of normally-distributed values themselves follow a normal distribution (of reduced standard deviation), but this is also very generally true even for non normally-distributed values, by virtue of the central limit theorem [13]. In materials science, the concept of "statistical significance" is closely related to that of (the size of) the representative volume element (RVE), and quantitative elements were presented by Kanit et al. [14] in the context of heterogeneous (or "composite") materials, but also previously discussed by, e.g., Huet [15]. Quoting Kanit et al. [14], "*The RVE is usually regarded as a volume V of heterogeneous material that is sufficiently large to be statistically representative of the composite, i.e., to effectively include a sampling of all microstructural heterogeneities that occur in the composite.*", and "*A RVE size can be associated with a given precision on the estimation of the wanted overall property [...]. It is shown to depend on the investigated morphological or physical property [...]*". When applied to polycrystals, this simply translates into the following fundamental points: *(i)* an RVE (for which statistical significance can be declared) can be defined as a number of grains; *(ii)* the RVE size is associated with the precision of a property (or "result"); and *(iii)* the precision depends on the property, or, in other terms, a specific number of grains provides different precisions for different properties, or, equivalently, different properties require different number of grains to be quantified to the same precision. For instance, in the case discussed previously, considering a statistical significance of the average at two standard errors, $\delta = 2\,\sigma_m$ (95% confidence), using Equation 1, the RVE size (n) is given by

$$n = \left(\frac{2\,\sigma}{\delta}\right)^2. \tag{2}$$

It follows from Equation 2 that greater statistical significance, which corresponds to a smaller δ value, demands a larger number of grains; for example, decreasing the error (δ) by a factor of 2 requires a four-fold increase to the number of grains (n).

These general concepts can be applied to the results reported in Ref. [1] to assess both their degrees of statistical significance and RVE sizes. In the case of average values, the precision and RVE sizes can be computed using Equations 1 and 2, and considering 95% confidence. In the case of distributions, the precision can only be estimated semi-quantitatively, in particular when they concern directions (e.g., distributions of rotation axes). Moreover, in contrast to the general case or the numerical application of Kanit et al. [14], where, e.g., the Young's moduli of several different (statistically-equivalent) polycrystals were computed to analyse their statistical significance, in the present experimental case, and for distributions, only the result on one polycrystal is available whose statistical significance must be analysed. This case was actually also discussed by Kanit et al. [14]: "*The [...] properties of random composites can be determined not only [...] on large volume elements of heterogeneous material, but also as mean values of apparent properties of*

rather small volumes, providing that a sufficient number of realizations is considered.", which corresponds to the ergodicity property [15]. It is therefore possible to consider subsets of the experimental data set to analyse their statistical significance and then infer on the statistical significance of the original data set, using Equations 1 and 2, as well as determine RVE sizes [14].

3 Application to experimental results

The experiment described in Ref. [1] provided results on the lattice rotations of 175 grains in a polycrystal deformed in plane strain compression to successive strains of 0.42, 0.77 and 1.2. In Ref. [11], the rotations were compared to those predicted by the Taylor model. The statistical significance of the main results reported in these works is analysed: the rotation angles (θ_0^ε and their evolutions), the rotation axes (r_0^ε), and the angle between the experimental and simulated rotation axes (α), which are all interpreted in terms of distribution or average over all grains. The complete results contains 157 grains for the rotation angles (after excluding grains subjected to orientation fragmentation [16]) and 123 for the rotation axes and α values (after further excluding those grains for which uncertainty on the rotation axis exceeds 20° [1,17]). Numerical analyses are done using Neper's post-processing capabilities [18,19].

3.1 Rotation angles (θ_0^ε)

The distributions over all grains of the rotation angles with respect to the initial orientations, θ_0^ε, are provided in Figure 1, and the associated description and conclusions were the following: "*The frequency distributions of the rotation angles θ_0^ε at successive strains are represented in [Figure 1]. As expected, they vary significantly from one grain to the other [...]. However, it appears that, as deformation increases, the rotation angles increase less: on average, they are 11° at $\varepsilon = 0.42$, 15° at $\varepsilon = 0.77$ and 18° at $\varepsilon = 1.2$.*" [1]. The statistical significance of the results and the validity of the conclusion can be analysed.

The distributions provided in Figure 1 do not exhibit high-frequency fluctuations and therefore apparently do not suffer from a lack of statistical significance. (This is simply due to the fact that the bin size of the distributions (6°) was chosen to avoid such fluctuations, which indirectly ensures that each bin has a representative number of grains). The standard errors of the average values can be computed using Equation 1, and the results are provided in Table 1. The average rotation angles are $\bar{\theta}_0^{0.42} = 10.9° \pm 0.87°$, $\bar{\theta}_0^{0.77} = 15.0° \pm 1.12°$ and $\bar{\theta}_0^{1.20} = 17.9° \pm 1.32°$ (95% confidence). The statistical significance of these results can be analysed in view of the conclusion made on the rotation trend, and the latter can be analysed more thoroughly from the changes of rotation angles between successive strains and normalized to exactly 0.4 strain, $\widehat{\Delta\theta}_0^\varepsilon$: $\widehat{\Delta\theta}_0^{0.42} = \theta_0^{0.42} \times 0.4/0.42$, $\widehat{\Delta\theta}_0^{0.77} = (\theta_0^{0.77} - \theta_0^{0.42}) \times 0.4/(0.77-0.42)$ and $\widehat{\Delta\theta}_0^{1.2} = (\theta_0^{1.2} - \theta_0^{0.77}) \times 0.4/(1.2-0.77)$. Their average values are $\overline{\widehat{\Delta\theta}_0}^{0.42} = 10.4° \pm 0.83°$, $\overline{\widehat{\Delta\theta}_0}^{0.77} = 4.6° \pm 0.66°$ and $\overline{\widehat{\Delta\theta}_0}^{1.20} = 2.7° \pm 0.44°$ (95% confidence). They decrease, and their confidence intervals do not overlap, which confirms the conclusion on the rotation trend. According to the values provided in Table 1, the conclusion is further confirmed to more than 99.7% confidence.

The RVE size can be defined as the minimal number of grains (n) for which the conclusion is valid, i.e. for which the confidence intervals do not overlap. Using the values provided in Table 1, the RVE size is obtained as follows (95% confidence):

$$10.4 - 2 \times \frac{5.2}{\sqrt{n}} \geq 4.6 + 2 \times \frac{4.1}{\sqrt{n}} \tag{3}$$

$$4.6 - 2 \times \frac{4.1}{\sqrt{n}} \geq 2.7 + 2 \times \frac{2.8}{\sqrt{n}}, \tag{4}$$

which yields a minimum value of $n = 53$ grains.

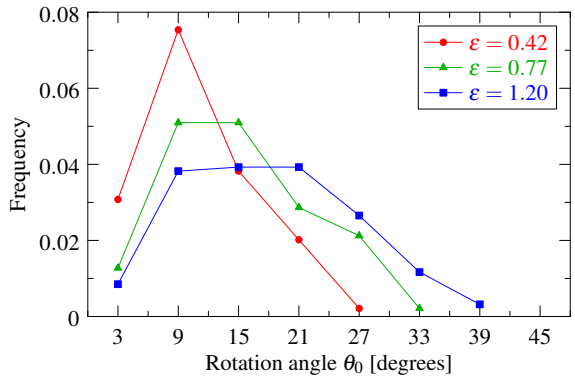

Figure 1: Rotation angles with respect to the initial orientations (θ_0^ε), at successive strains.

Strain range	$\bar{\theta}$ (°)	σ (°)	σ_m (°)	$\bar{\theta} \pm \sigma_m$ (°) (68% confidence)	$\bar{\theta} \pm 2\,\sigma_m$ (°) (95% confidence)	$\bar{\theta} \pm 3\,\sigma_m$ (°) (99.7% confidence)
0 to 0.42	10.9	5.5	0.44	10.9 ± 0.44	10.9 ± 0.87	10.9 ± 1.31
0 to 0.77	15.0	7.0	0.56	15.0 ± 0.56	15.0 ± 1.11	15.0 ± 1.67
0 to 1.20	17.9	8.2	0.66	17.9 ± 0.66	17.9 ± 1.31	17.9 ± 1.97
0 to 0.42 *	10.4	5.2	0.42	10.4 ± 0.42	10.4 ± 0.83	10.4 ± 1.25
0.42 to 0.77 *	4.6	4.1	0.33	4.6 ± 0.33	4.6 ± 0.66	4.6 ± 0.99
0.77 to 1.20 *	2.7	2.8	0.22	2.7 ± 0.22	2.7 ± 0.44	2.7 ± 0.66

Table 1: Statistics on the rotation angles with respect to the initial orientation (θ_0^ε), and their changes between successive strains ($\widehat{\Delta\theta}_0^\varepsilon$, indicated by an asterisk). $\bar{\theta}$ and σ are the average and standard deviation of the distribution, respectively, and σ_m is the standard error of the average.

3.2 Rotation axes (r_0^ε)

The distributions over all grains of the rotation axes are provided in Figure 2, and the associated description and conclusions were the following: "*The distributions of the rotation axes r_0^ε are illustrated in [Figure 2] by pole figures which are reduced to one-quarter using the orthotropic symmetry. Each axis is represented by a point and a density function is constructed by associating a Gaussian spread of half-width 7° to each axis. The axes appear to be preferentially distributed about TD at the first increment (density = 5), and then about an axis located between TD and ND, more precisely* $[0.83 \times TD + 0.56 \times ND]$ *(density = 3).*" [1]. The axes are RD (the "rolling direction"), TD (the "transverse direction") and ND (the "normal direction"). The statistical significance of the dominant TD component at low strain and of the transition from TD to TD–ND during deformation can be analysed.

As explained in Section 2, several subsets of the original data set are considered. A number of 10 half-sized subsets, which contain 61 or 62 grains, are generated by random sampling of the original data set, and, for each subset, its complement is also considered, leading to a total of 20 subsets. The main interest of considering subsets and their complements is that they provide independent data, which is a base assumption in the theory leading to Equations 1 and 2 (of course, this is only the case for a subset and its complement, not for subsets corresponding to different samplings).

The results of four representative subsets are provided in Figure 3, while (for reasons of space) the full array of results is provided in Supplementary Material. Three of the subsets (cases a–c) provide the same trends as the original set (Figure 2), despite stronger local fluctuations resulting from the smaller number of grains. Case d, in contrast, exhibits a clear dominant TD component at low strains but not a very clear transition from TD to TD–ND during deformation. Among the 20 subsets analysed, 18 showed a clear dominant TD component at low strains, and 13 also showed a clear transition from TD to TD–ND during deformation. For $n = 61$–62, the dominant TD component is therefore ascertained to about 90% confidence, and the transition to TD–ND to about 65% confidence. The nature of the result does not easily allow for a fully quantitative analysis, but the standard case of a normally-distributed error can be considered to get an idea of the statistical significance of the original data set and of the RVE sizes. 90% confidence corresponds to a $\pm 1.64\,\sigma$ interval, and 60% to a $\pm 0.94\,\sigma$ interval. According to Equation 2, this would lead to greater errors on the original data set by a factor of $\sqrt{2}$, which corresponds to $\pm 2.3\,\sigma$ and $\pm 1.33\,\sigma$ intervals, respectively, which in turn correspond to 98% and 81% confidence, respectively. Using the same approach, tentative RVE sizes are obtained for 95% confidence and are $n \simeq 90$ grains for the dominant TD component at low strains and $n \simeq 280$ grains for the TD to TD–ND transition at large strains.

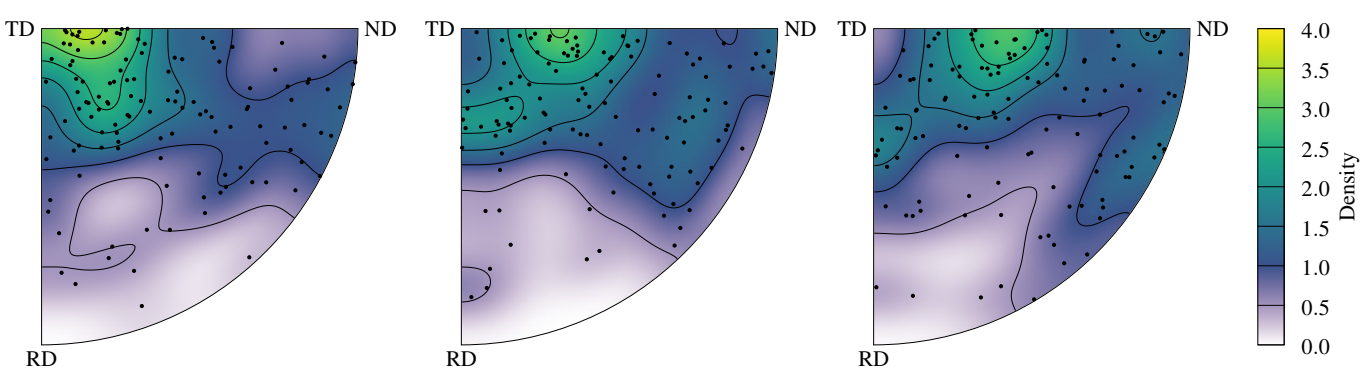

Figure 2: Rotation axis ($\boldsymbol{r}_0^\varepsilon$) distributions at $\varepsilon = 0.42$, $\varepsilon = 0.77$ and $\varepsilon = 1.2$ (from left to right), represented as equal-area projections. Compared to Ref. [1], the intensities are slightly different, which is due to a (uniform) normalization correction.

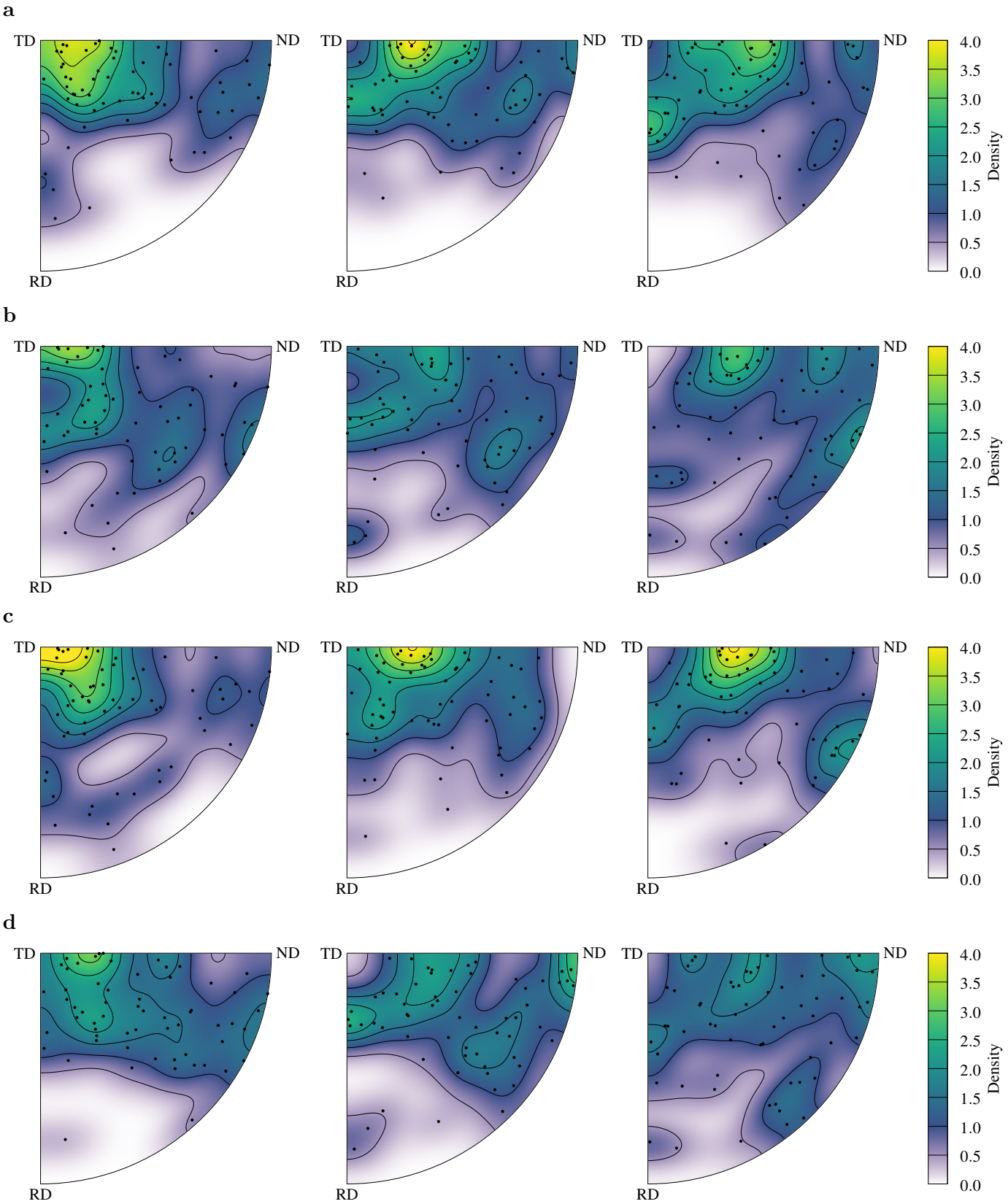

Figure 3: Rotation axis ($\boldsymbol{r}_0^{\varepsilon}$) distributions at $\varepsilon = 0.42$, $\varepsilon = 0.77$ and $\varepsilon = 1.2$ (from left to right) for four different subsets containing 61 or 62 grains, represented as equal-area projections. Cases a and b are complementary sets and therefore represent independent data, so as cases c and d.

3.3 Correlation between the experimental and simulated rotation axes (α)

The distributions over all grains of the angles between the experimental rotation axes and those predicted by the Taylor model, α between $\boldsymbol{r}^{\text{exp}}$ and $\boldsymbol{r}^{\text{pred}}$, are provided in Figure 4, and the associated description and conclusions were the following: "*The correlation between the rotation axes is investigated in [Figure 4]. It is quantified for each grain in terms of the angle α between the experimental axis $\boldsymbol{r}^{exp}$ and the predicted axis $\boldsymbol{r}^{pred}$. [...] whatever the increment, the α angles tend to be relatively small. For example, at the first increment, the average value of α is 39° (against 90° for uncorrelated axes), which denotes quite a strong correlation between the experimental and predicted axes. Hence, the Taylor model provides a so-called 'first-order agreement' for the rotation axes.*" [11]. The statistical significance of the average value of α and the validity of the conclusion can be analysed.

As in the case of the rotation angle, it can first be observed that the distributions themselves do not exhibit high-frequency fluctuations (for the same reason, owing to the choice of the bin size) and therefore apparently do not suffer from a lack of statistical significance. The standard error on the average value of α at the first increment (39°) can be computed using Equation 1 (with $n = 123$), which yields $\sigma_m = 30/\sqrt{123} \simeq 2.7°$; the precision on the average is therefore equal to 5.4° (95% confidence). It is fair to consider that the conclusion could have be drawn for any α value in the interval $39 \pm 5.4°$, and therefore the result can be considered as statistically significant. The relatively large absolute uncertainties are also to compare with those on the measured rotation axes, which themselves are only defined to several degrees [1]. RVE sizes can be computed using Equation 2 for given precisions and are equal to 36 grains for $\delta = 10°$, 57 grains for $\delta = 8°$, 74 grains for $\delta = 7°$ and 100 grains for $\delta = 6°$ (95% confidence).

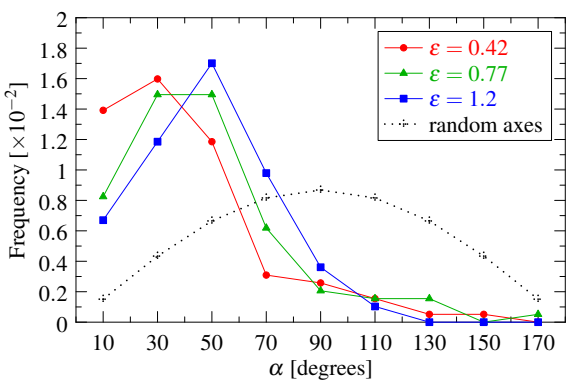

Figure 4: Grain-by-grain comparisons of the rotation axes for the three strain increments. α is the angle between the experimental and Taylor model rotation axes ($\boldsymbol{r}^{\text{exp}}$ and $\boldsymbol{r}^{\text{pred}}$, respectively).

4 Conclusions

The statistical significance of the main results of Refs. [1,11] could be analysed quantitatively using simple elements of the theory of statistics, and RVE sizes (as number of grains) could be determined. It was found that the different results are defined to different precisions, and that getting the same level of precision on the different results would require different RVE sizes. Concerning the statistical significance, the following conclusions could be drawn:

- The values of the average rotation angles (θ_0^ε) are defined to well below 1° (at 95% confidence), and the conclusion is valid to more than 99.7% confidence;
- The different properties of the distributions of the rotation axes are confirmed to different degrees: the dominant TD component at low strains is confirmed to 98% confidence and the transition from TD to

TD–ND directions during deformation is confirmed to 81%;

- The analysis of the correlation between the experimental rotation axes and the rotation axes predicted by the Taylor model is confirmed to about 5°, at $\alpha = 39° \pm 5°$, which validates the conclusion on a "first-order agreement" between the experimental and predicted rotation axes.

Concerning the RVE sizes, the following conclusions could be drawn (95% confidence):

- The analysis of the rotation angles and the conclusion on their evolutions during deformation require 53 grains;
- A clear definition of the dominant TD component of the rotation axis distribution requires about 90 grains, and a clear definition of the transition from TD to TD–ND directions during deformation requires about 280 grains;
- The correlation between the experimental and predicted rotation axes (average value of α) requires a few tens to 100 grains, depending on the precision, from 36 grains for $\delta = 10°$ to 100 grains for $\delta = 6°$.

So, while average values are defined to the greatest precision and require relatively few grains to establish trends, the distributions of rotation axes are the ones requiring the greater number of grains, especially when it comes to analysing evolutions during deformation.

Overall, the analysis confirms the statistical significance of the results provided in Refs. [1, 11], and effectively corrects the assertion made in Ref. [10] and recalled in Introduction. Actually, reasonable arguments why Refs. [1, 11] and [2] reported different conclusions on the agreement between experiment and Taylor model simulation were discussed in Ref. [1] and mainly concern the experimental and observation conditions; the interested reader may also refer to Refs. [16, 20] (and [21–23]) regarding further developments on the experimental data presented in Ref. [1], especially in relation to other elements of Ref. [10] not discussed in this article.

To conclude, it can be considered that fundamental results on the grain-scale rotations in typical aluminium alloys can generally be obtained using a few tens to a couple hundreds grains. Using a significantly larger number of grains is of course interesting to improve the statistical significance (reduce standard errors), but is even more useful to pursue investigations that would otherwise remain out-of-reach. In this article, it was shown that the precision and RVE size (necessary number of grains) depend on the result of interest, but they are also expected to depend, to some degree, on the material and deformation conditions. The proposed method is general and can be applied to data sets obtained in different conditions to determine their own precisions and RVE sizes.

5 Data availability

The data are openly available at https://tel.archives-ouvertes.fr/tel-00414120v3.

6 Acknowlegments

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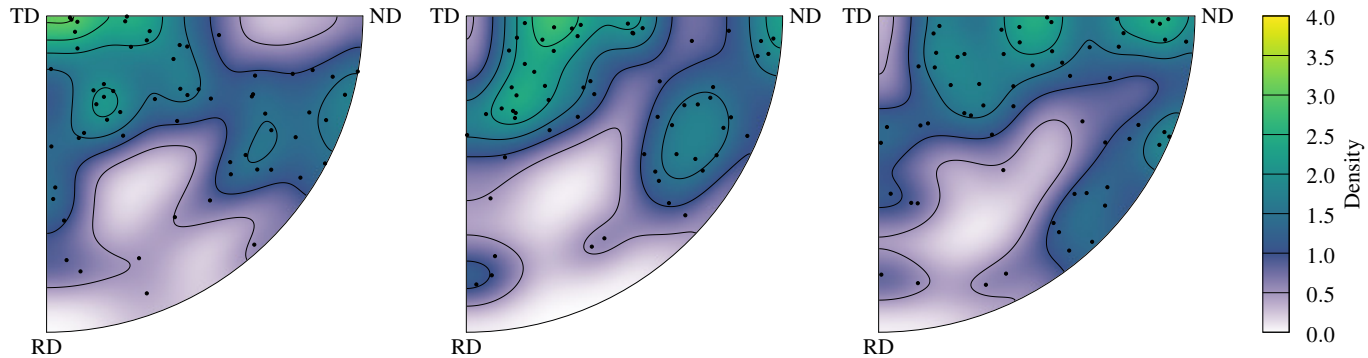
Supplementary material

The rotation axis distribution of 20 subsets containing 61 or 62 grains are provided in Figure 1. For each subset, the distributions correspond to strains of 0.42, 0.77 and 1.2, from left to right. Subsets are complement sets by pair (subsets 1 and 2, subsets 3 and 4, etc.). Each pair therefore provide two independent data sets. The distributions are analysed with respect their showing *(i)* a clear dominant TD component and *(ii)* a clear transition of the dominant component from TD to TD–ND during deformation. The results are reported in Table 1.

Subset 1



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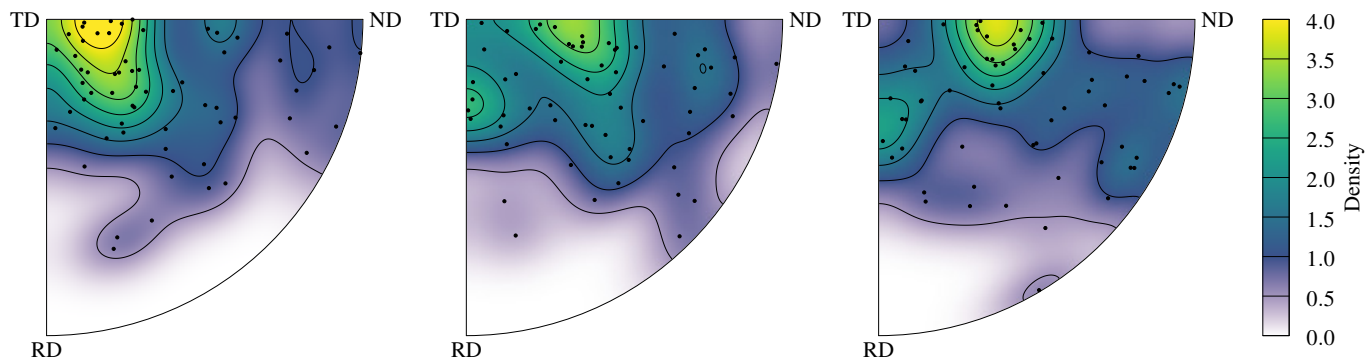


Subset 3

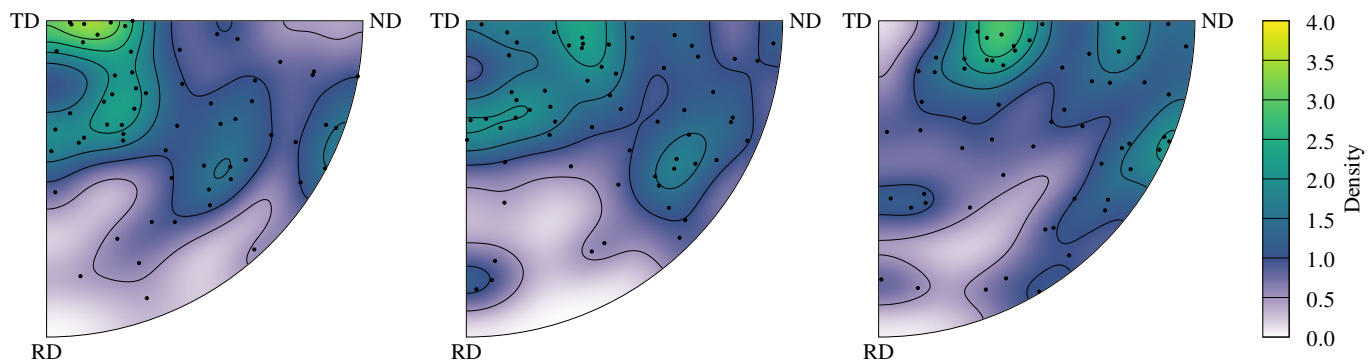
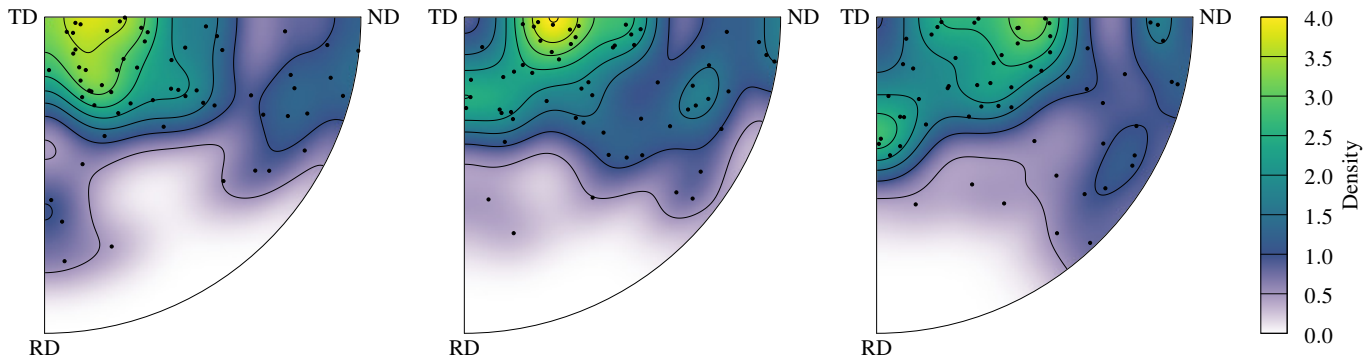
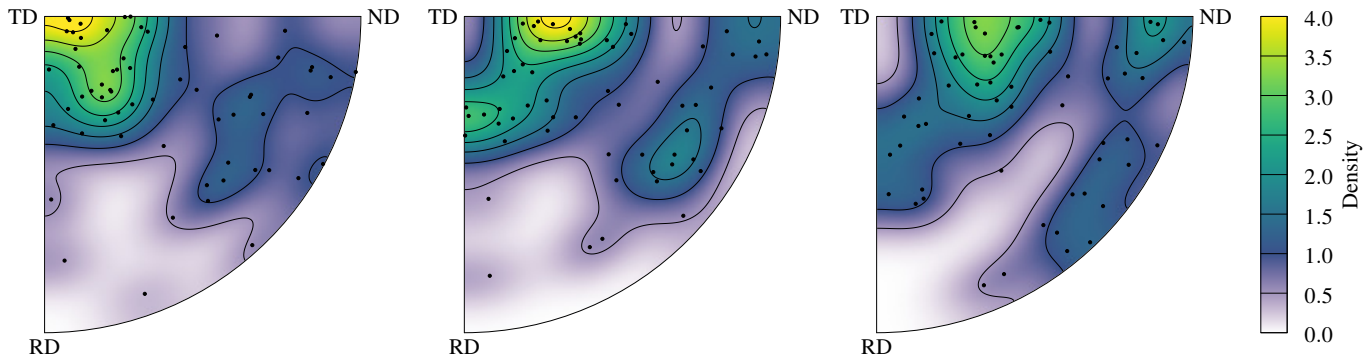


Figure 1: Rotation axis ($\boldsymbol{r}_0^{\varepsilon}$) distributions at $\varepsilon = 0.42$, $\varepsilon = 0.77$ and $\varepsilon = 1.2$ (from left to right), represented as equal-area projections for 20 different subsets containing 61 or 62 grains.

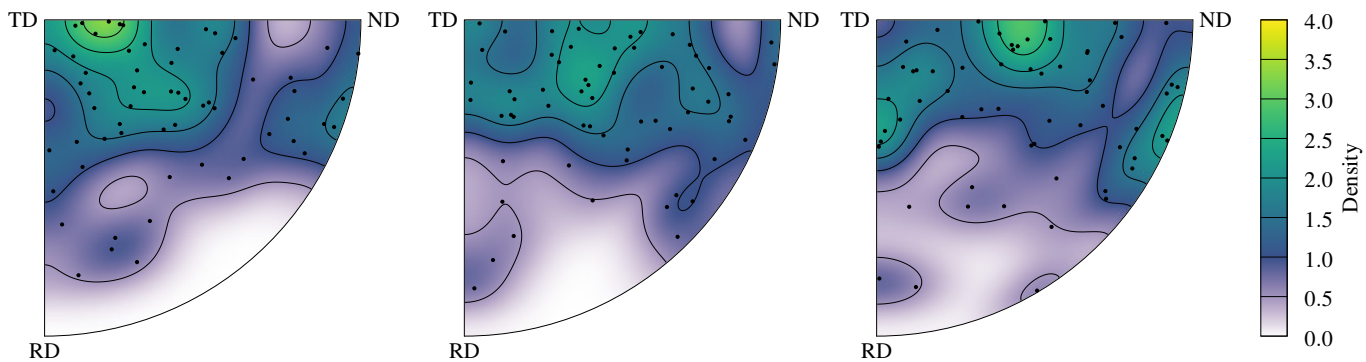
Subset 4



Subset 5



Subset 6



Subset 7

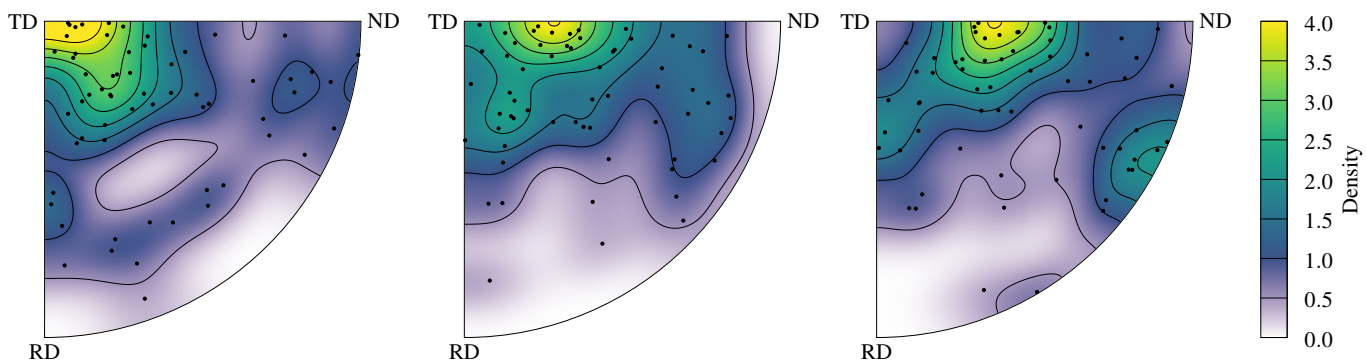
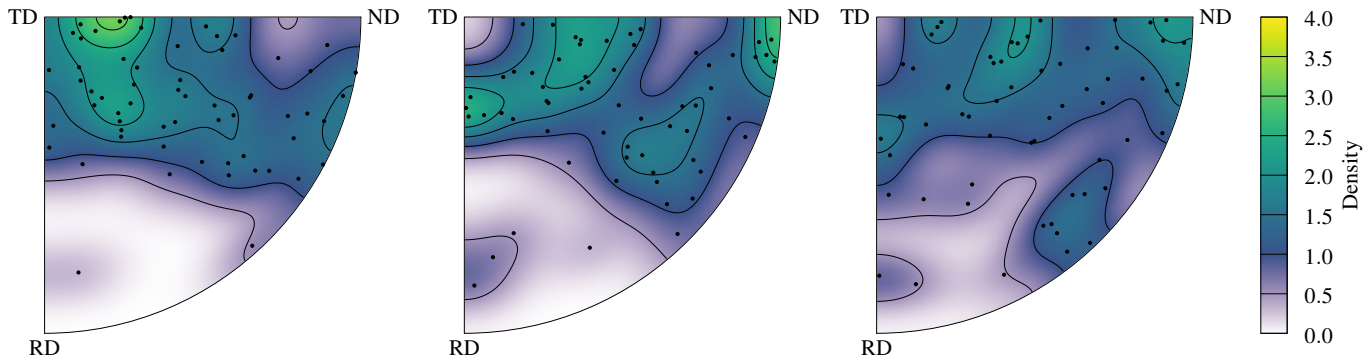
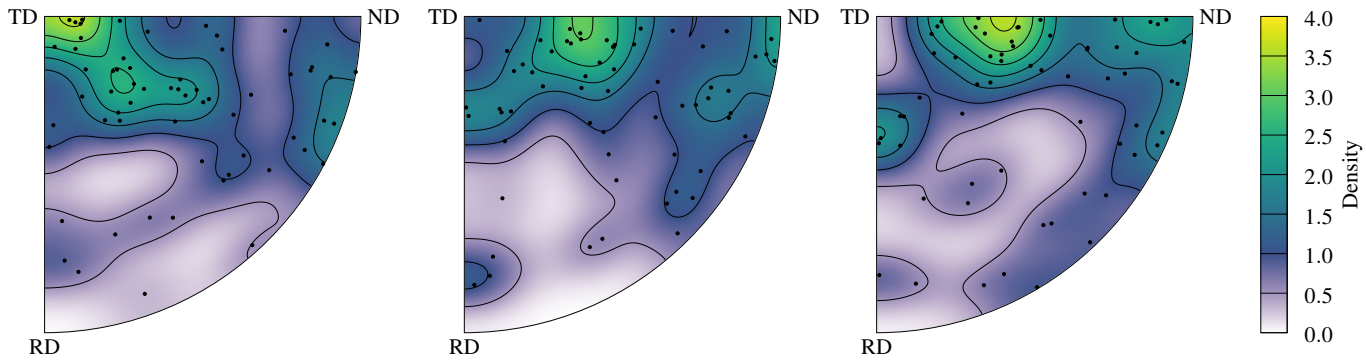


Figure 1: (continued)

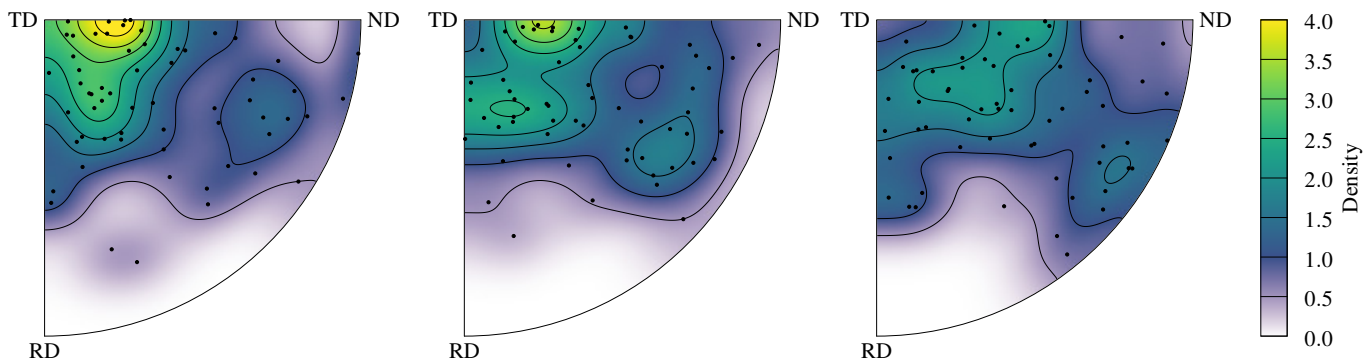
Subset 8



Subset 9



Subset 10



Subset 11

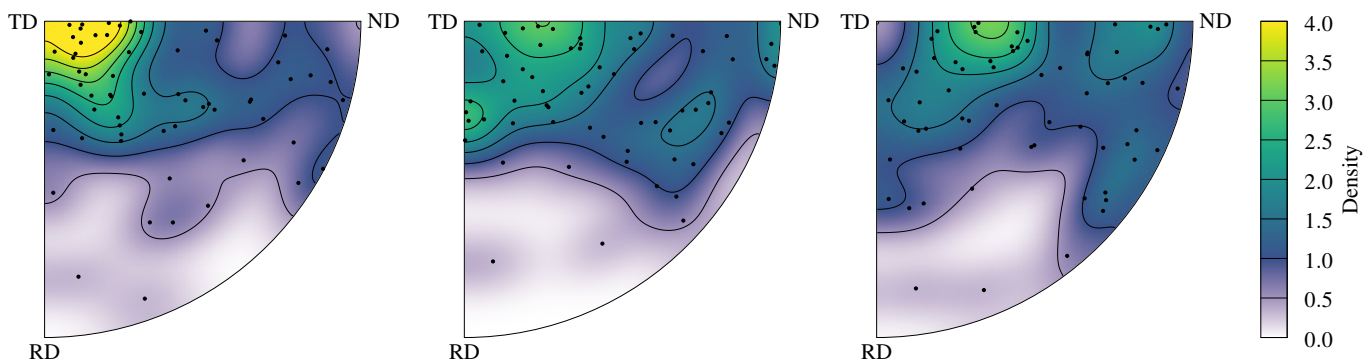
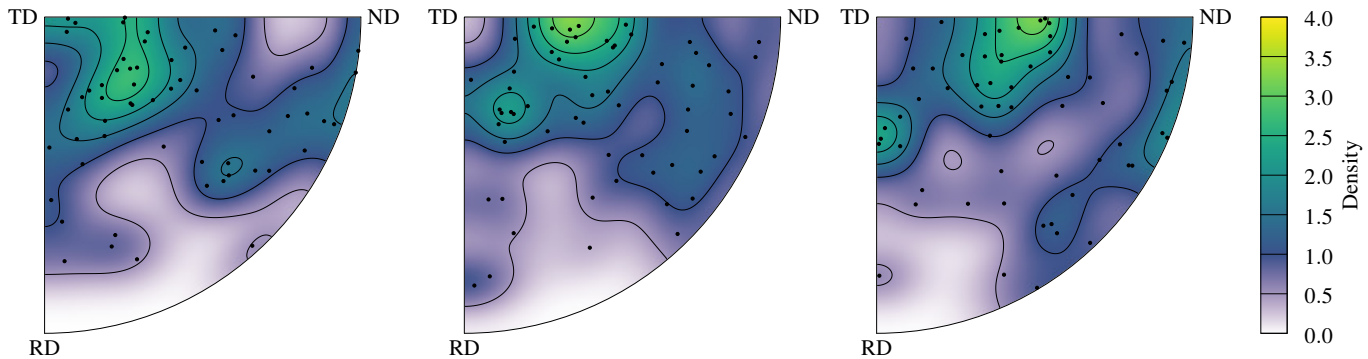
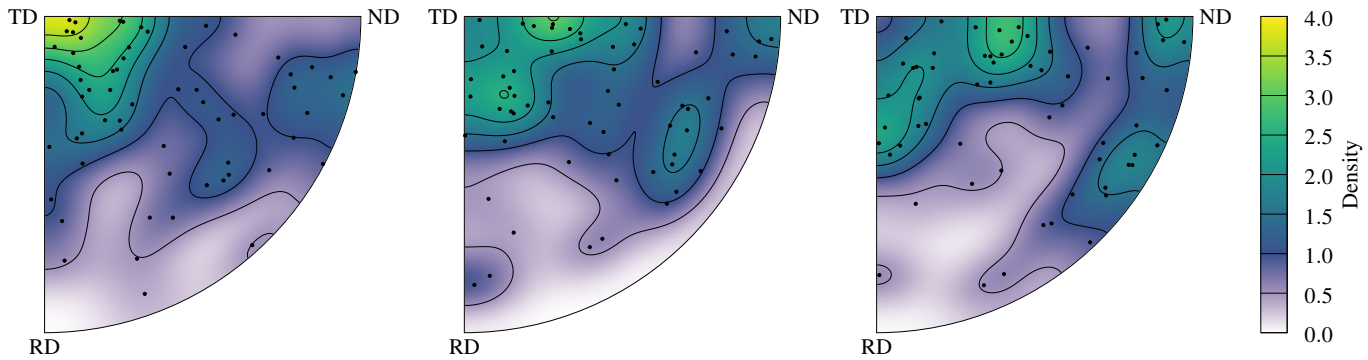


Figure 1: (continued)

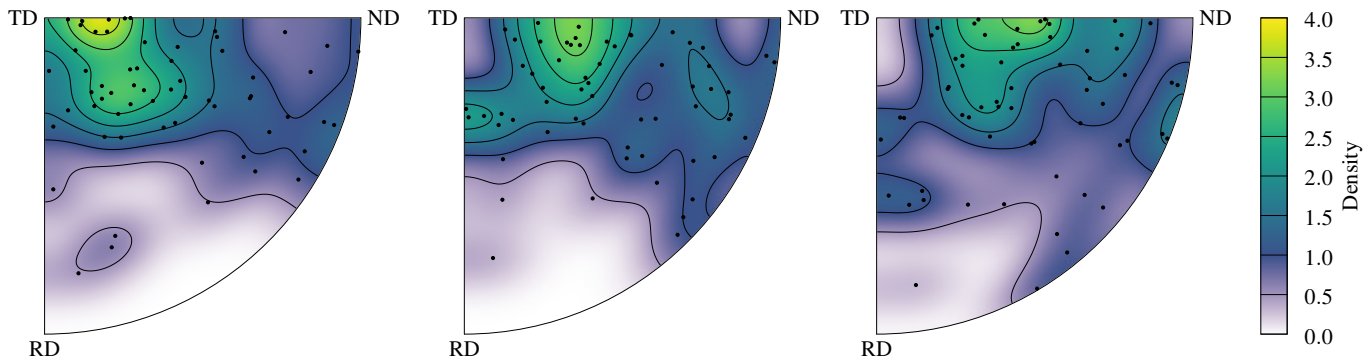
Subset 12



Subset 13



Subset 14



Subset 15

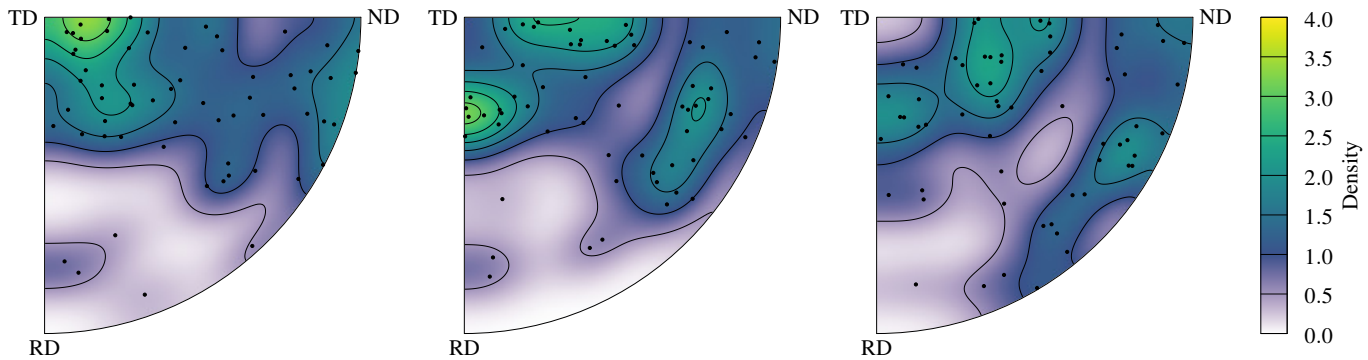
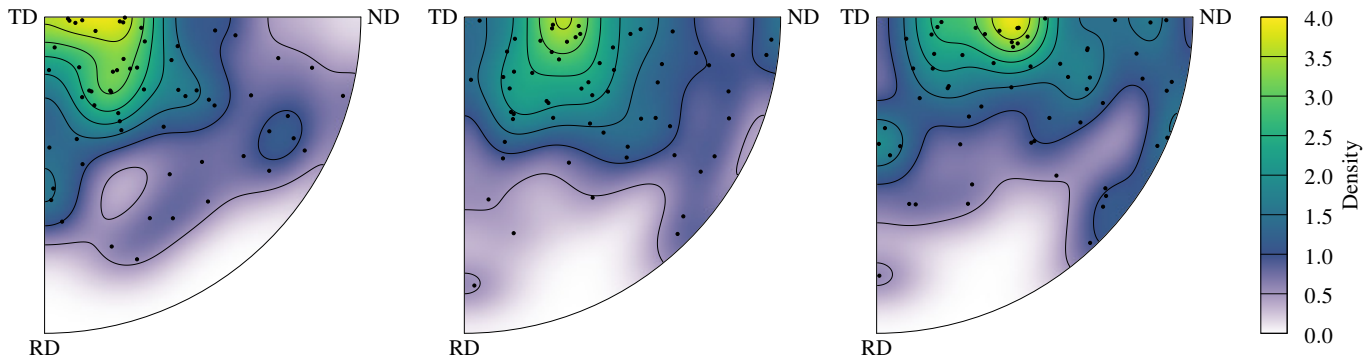
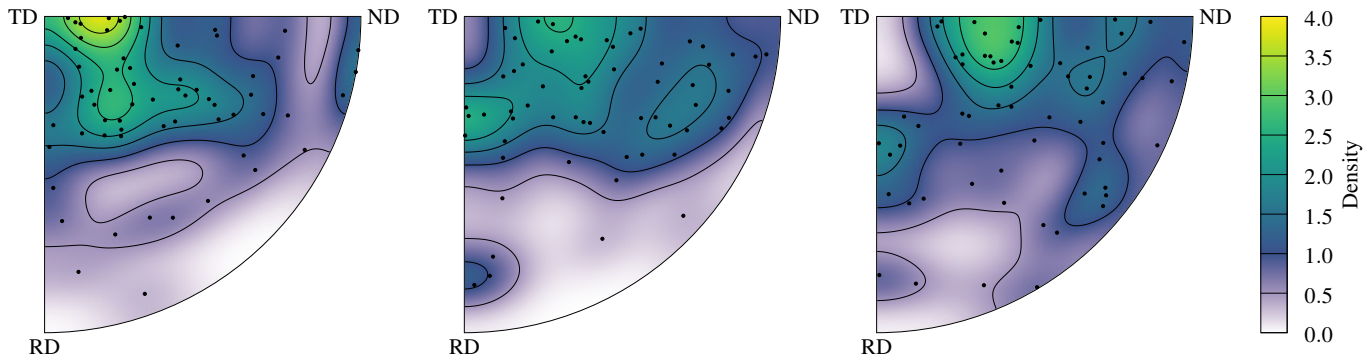


Figure 1: (continued)

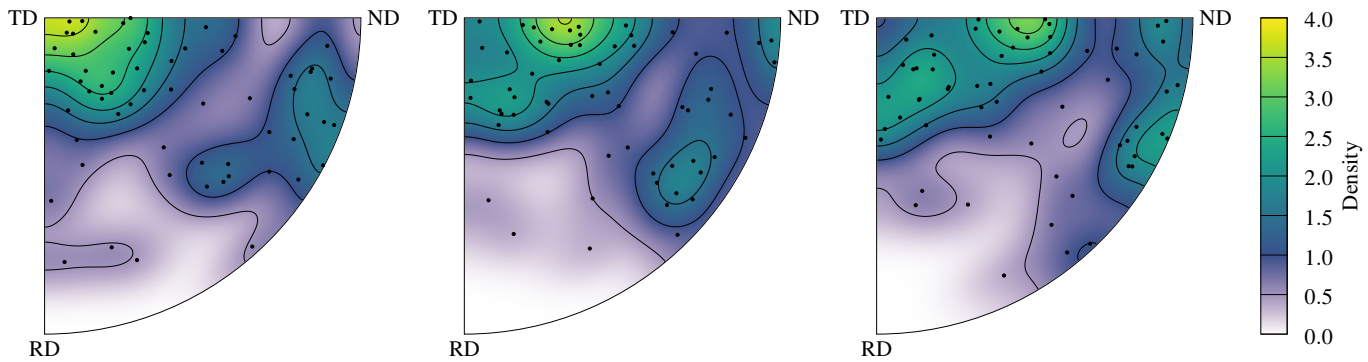
Subset 16



Subset 17



Subset 18



Subset 19

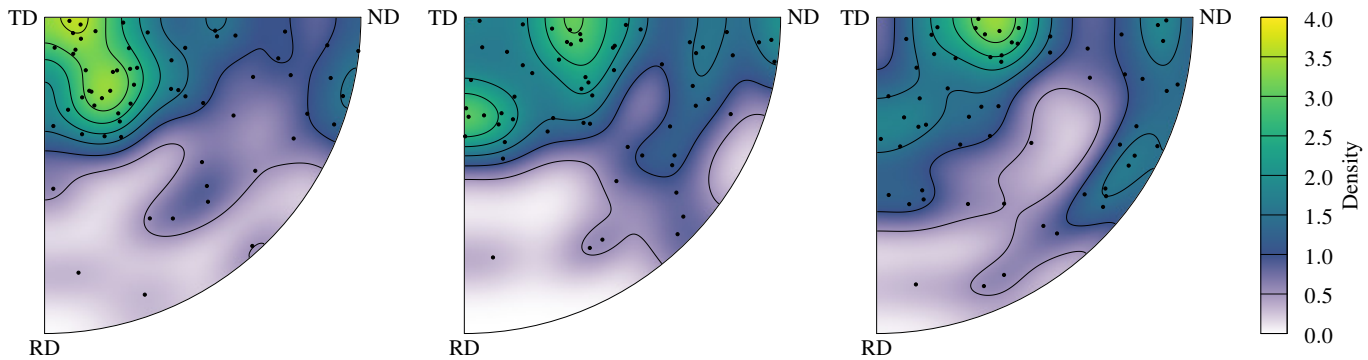


Figure 1: (continued)

Subset 20

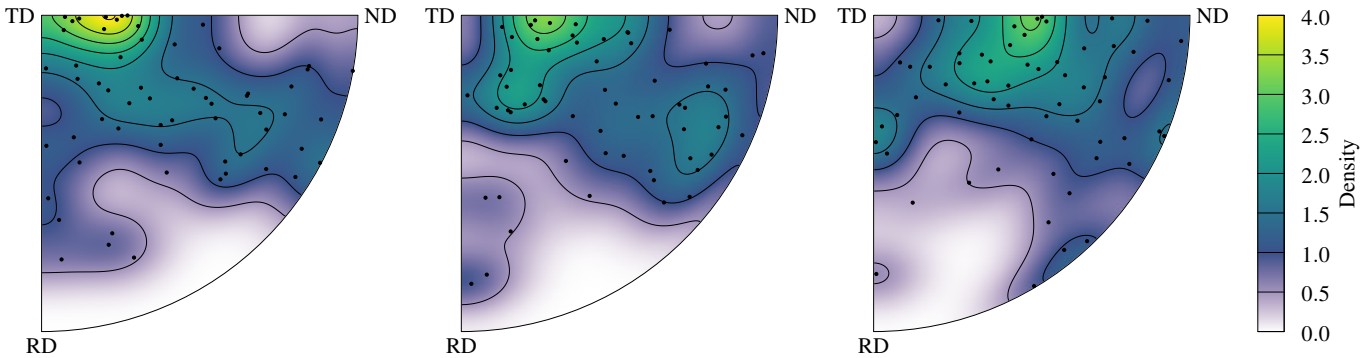


Figure 1: (continued)

Subset	Clear dominant TD	Clear transition from TD to TD–ND
1	no	no
2	yes	yes
3	yes	no
4	yes	yes
5	yes	yes
6	yes	no
7	yes	yes
8	no	no
9	yes	yes
10	yes	no
11	yes	yes
12	yes	yes
13	yes	no
14	yes	yes
15	yes	no
16	yes	yes
17	yes	yes
18	yes	yes
19	yes	yes
20	yes	yes

Table 1: Properties of the rotation axis distribution of the 20 subsets, in terms or clear or unclear dominant TD component at low strains and clear or unclear transition from TD to TD–ND during deformation.