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► **To cite this version:**

S. Hémerly, P. Villechaise. In situ EBSD investigation of deformation processes and strain partitioning in bi-modal Ti-6Al-4V using lattice rotations. *Acta Materialia*, 2019, 171, pp.261-274. 10.1016/j.actamat.2019.04.033 . hal-02166762

**HAL Id: hal-02166762**

**<https://hal.science/hal-02166762>**

Submitted on 22 Oct 2021

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# 1 In situ EBSD investigation of deformation processes and strain partitioning in bi-modal Ti-6Al-4V 2 using lattice rotations

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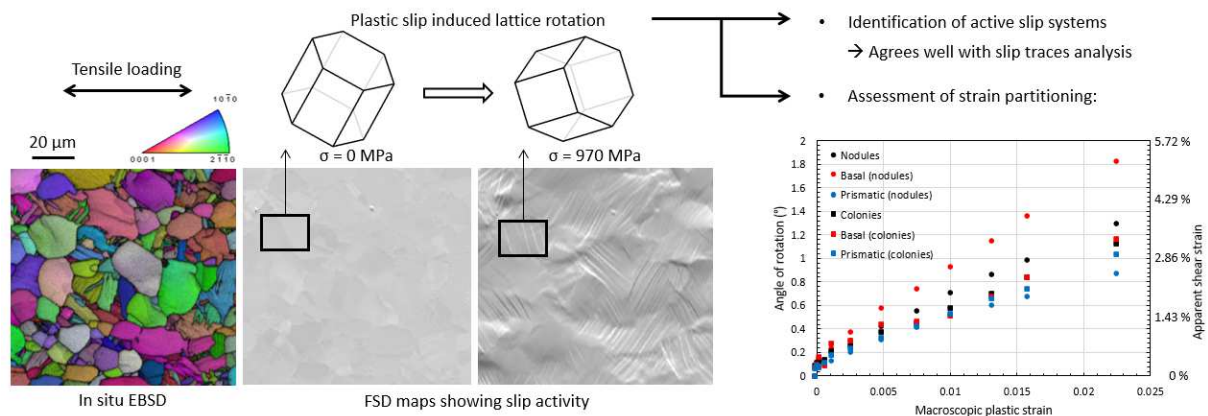
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## 8 Abstract

10 Identification of operating deformation processes and assessment of the resulting strain  
11 partitioning are critical concerns for mechanical properties prediction and microstructure  
12 optimization in complex alloys such as  $\alpha/\beta$  titanium alloys. Lattice rotation relative to the initial  
13 orientation was presently used as a marker of slip activity. A Ti-6Al-4V specimen with a bi-modal  
14 microstructure was tested in tension in a scanning electron microscope. Crystallographic orientations  
15 were characterized in situ using electron back-scattered diffraction (EBSD). A successful prediction of  
16 activated slip systems was achieved using the rotation axis associated with plastic activity. The  
17 combination of this procedure and slip traces analysis offers an insight into the determination of  
18 both slip plane and slip direction of active slip systems. Based on classical crystal plasticity  
19 formulations, the magnitude of the rotation relative to the initial orientation was interpreted in  
20 terms of plastic shear magnitude. A quantitative assessment of plastic strain at the microstructure  
21 scale was then carried out using lattice rotation data. This approach enabled to discuss strain  
22 partitioning in Ti-6Al-4V considering the influence of microstructural features and active slip modes.

23

## 24 Graphical abstract:



25

26 **Keywords:** Titanium alloys; EBSD; Slip; Grain rotation; Strain distribution

27

## 28 1. Introduction

29  $\alpha / \beta$  titanium alloys are widely employed in the aerospace industry owing to superior  
30 mechanical properties. In particular, bi-modal microstructures composed of equiaxed primary  $\alpha$   
31 nodules and colonies of secondary  $\alpha$  lamellas embedded in the  $\beta$  matrix are extensively employed.

32 This duplex microstructure combines the advantages of equiaxed and lamellar structures for a well-  
33 balanced property profile [1]. The thermo-mechanical processing route determines the  
34 microstructural features [2]. In-service properties notably depend on (i)  $\alpha$  precipitates arrangements,  
35 morphologies, sizes and associated volume fractions [3,4], (ii) crystallographic textures [5,6] and (iii)  
36 elemental partitioning, short-range ordering and  $\alpha_2$  precipitation [7,8]. Tailoring of microstructure for  
37 optimum performance is looked for through a thorough understanding of the operative deformation  
38 and damage processes in relation with microstructural characteristics.

39 The duplex microstructure of titanium alloys induces a heterogeneous plastic deformation  
40 behavior. According to in situ scanning electron microscopy observations of tensile deformation, the  
41 early slip activity proceeds in nodules [9-13]. In order to obtain a good match between crystal  
42 plasticity simulations and experimental observations, a higher critical resolved shear stress value is  
43 usually assigned to colonies, which testifies of a delayed slip activity in transformed  $\beta$  regions [14,15].  
44 This spatially heterogeneous character is amplified by the intrinsic plastic anisotropy of the  
45 hexagonal close-packed  $\alpha$  phase. Different strengths were reported for the various families of slip  
46 systems [16-18]. While basal and prismatic slip strengths, which have been recently reviewed in [4],  
47 are similar, the pyramidal slip strength is significantly higher. However, only the latter mode can  
48 accommodate the c-axis deformation of the hexagonal close-packed lattice. As a result, the overall  
49 response of titanium alloys is governed by stress and strain partitioning, which has been identified as  
50 a key phenomenon under monotonic tension, fatigue or dwell-fatigue loadings for instance [17,19-  
51 21]. However, experimental data including a quantitative assessment of the heterogeneities are still  
52 scarce.

53 Electron backscatter diffraction (EBSD) is a common laboratory based tool used to measure  
54 crystal orientations from crystalline samples [22]. Various EBSD based procedures have been  
55 proposed to analyze plastic strain at the microstructure scale [23,24]. Degradation of the diffraction  
56 patterns in strained materials was first used as an indication of the distribution of strain [25].  
57 Alternatively, a local misorientation based approach, which relies on the variation of crystal  
58 orientation within a grain, was introduced as strain estimation procedure [26-28]. Local plastic  
59 deformation processes were also studied using the lattice rotation relative to its initial orientation.  
60 The rotation path was found characteristic of activated slip systems [29-31]. Although no strain  
61 quantification was attempted, a prior study reported a linear relationship between macroscopic  
62 plastic strain and lattice rotation using X-ray diffraction [29,32]. Analytically, the rate of reorientation  
63 of the crystal axes  $\mathbf{W}^*$  is decomposed as follows [33]:

$$64 \quad \mathbf{W}^* = \mathbf{W}^g - \mathbf{W}^c \quad (1)$$

65 With  $\mathbf{W}^g$  the 'rigid-body spin' describing the grain shape rotation relative to a reference frame and  
66  $\mathbf{W}^c$  the plastic spin describing the differential rotation of the samples axes of a grain in terms of its  
67 crystallographic axis. Individual assessment of both rotation components is experimentally  
68 challenging.  $\mathbf{W}^g$  can be decomposed into a component accounting for the sample rotation relative to  
69 the reference frame and a component relative to the grain shape rotation relative to the sample  
70 frame. The contribution of the former component can be limited through carefully controlled test  
71 conditions. For instance, in situ testing limits specimen positioning error at each deformation step.  
72 Material homogeneity at the specimen scale is also an important factor. The latter component,  
73 accounting for grain shape rotation relative to the sample frame, is the consequence of the  
74 deformation of surroundings. This effect, which is also difficult to evaluate, could be dismissed using  
75 a statistical approach. The effect of deforming neighbors should compensate provided multiple  
76 grains are considered. Finally,  $\mathbf{W}^c$  is expressed for an elementary volume in most crystal plasticity  
77 models using equation (2) [33]:

78 
$$W^c = \sum_{i=1}^N \frac{1}{2} (\mathbf{s}_i \otimes \mathbf{m}_i - \mathbf{m}_i \otimes \mathbf{s}_i) \dot{\gamma}_i \quad (2)$$

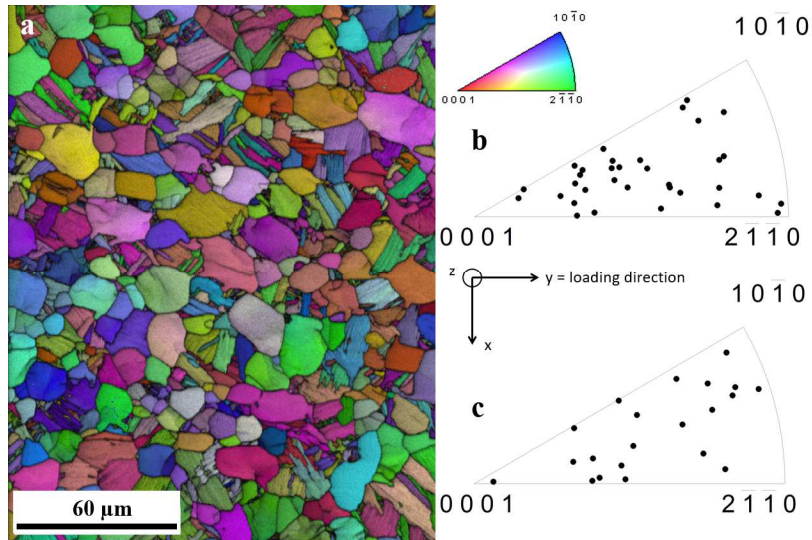
79 With  $\dot{\gamma}_i$  the slip rate,  $\mathbf{s}_i$  the slip plane in the sample frame and  $\mathbf{m}_i$  the slip direction in the  
80 sample frame associated with slip system  $i$ . If a single slip system is active, the following remarks can  
81 be made using equation (2). Firstly, the axis of the lattice rotation rate is characteristic of the  
82 activated slip system. Secondly, the predicted lattice rotation rate magnitude is directly proportional  
83 to the plastic shear rate. Therefore, a straightforward relation between experimentally measured  
84 lattice rotation and plastic shear can be found if appropriate test conditions and procedures are  
85 applied. The present work is based on this analysis.

86 In this article, we introduce a novel approach to study plastic deformation and strain  
87 partitioning based on in situ electron back-scattered diffraction (EBSD) characterization of lattice  
88 rotation during a tensile test. The lattice rotation relative to the initial orientation is used as a source  
89 of information on deformation behavior at the grain scale. A procedure for active slip system  
90 identification is first proposed and discussed regarding slip traces analysis as a reference procedure.  
91 The relation between plastic strain and lattice rotation in terms of magnitude is then discussed based  
92 on experimental data and analytical calculations. This analysis is finally used to assess the respective  
93 influence of microstructural features and active slip modes on strain partitioning. Improvements in  
94 the understanding and modeling of deformation of bi-modal Ti-6Al-4V are discussed.

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## 96 2. Experimental

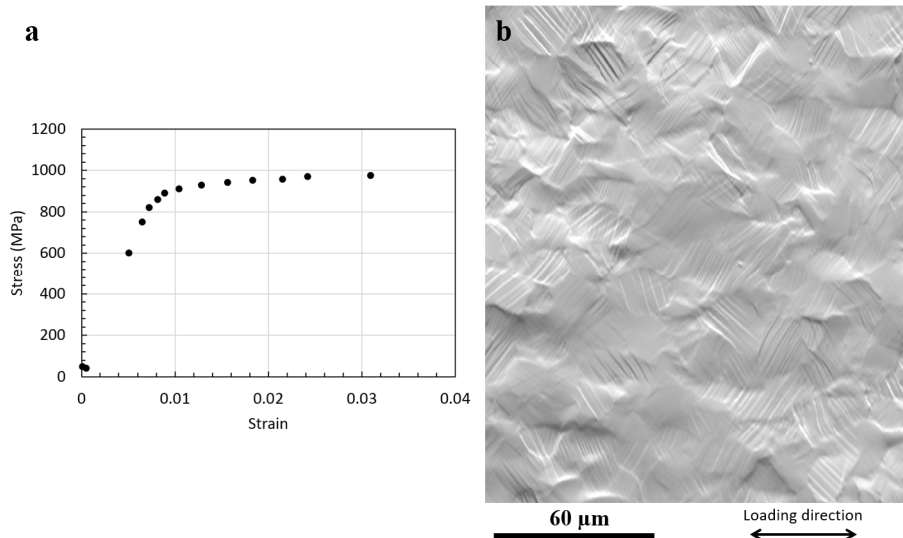
97 Ti-6Al-4V with a bimodal microstructure composed of equiaxed primary  $\alpha$  nodules and  
98 secondary  $\alpha$  lamellas embedded in the  $\beta$  matrix is used in the present study. According to EBSD  
99 analysis, primary  $\alpha$  nodules with an average diameter of 12  $\mu\text{m}$  account for 54 % of the specimen  
100 surface. The microstructure and the local crystallographic orientations in the region followed in situ  
101 are presented in figure 1 a. In this alloy, the  $\beta$  phase is associated with a low surface fraction [9]. As a  
102 consequence, only  $\alpha$  phase was considered. 34 primary  $\alpha$  nodules and 21 lamellar colonies were  
103 selected for the present investigations. The nodules exhibit an average diameter of about 12  $\mu\text{m}$ . The  
104 set of colonies was built to obtain a similar average diameter. The grain averaged crystallographic  
105 orientations are plotted on an inverse pole figure in figure 1 b and 1 c for the 34 nodules and the 21  
106 colonies respectively. The crystallographic orientations are fairly well distributed over the whole  
107 orientation domain for both nodules and colonies. Since the different slip modes are favored in  
108 distinct crystallographic orientation domains [9], a similar distribution of basal and prismatic slip  
109 modes is expected for both nodules and colonies.



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111 **Figure 1. a. Image quality and inverse pole figure along the loading direction showing the microstructure and**  
 112 **the crystallographic orientation in the region of interest (the loading direction is horizontal), b. and c. inverse**  
 113 **pole figure plots showing the average crystallographic orientations of nodules and colonies considered in the**  
 114 **present study**

115 An *in situ* tensile test was carried out using a Deben tensile stage with a 2 kN loadcell in a  
 116 JEOL 6100 scanning electron microscope (SEM) equipped with an EBSD setup provided by EDAX. A  
 117 0.8 mm thick dogbone shaped specimen with a gage length of 10 mm and a gage width of 2 mm was  
 118 used. After grinding both faces up to 4000 grade SiC paper, two additional polishing steps were  
 119 applied on one face. Rough polishing was carried out using a solution containing 9 μm diamond  
 120 particles. A final polishing step was applied using a mixture of colloidal silica suspension with a mean  
 121 particle size of 0.04 μm and 10 % H<sub>2</sub>O<sub>2</sub>. Incremental loading of the specimen was performed using a  
 122 displacement rate of 0.02 mm min<sup>-1</sup>. The crosshead displacement is measured using a linear variable  
 123 differential transformer position transducer. The engineering strain is derived from the displacement  
 124 data after a machine stiffness correction using a reference Young's modulus of 115 GPa. In order to  
 125 characterize the surface of the specimen at different deformation stages, the crosshead  
 126 displacement was stopped after reaching targeted stress values. The engineering stress – strain  
 127 conditions corresponding to arrests of the crosshead displacement are plotted on figure 2a. The  
 128 characterization of the crystallographic orientations in the region of interest was performed at each  
 129 stop using EBSD. The microscope is operated under a 25 kV tension and a probe current of about 5  
 130 nA is used. Kikkuchi diffraction patterns are acquired with a 5 x 5 binning (128 x 96 pixels) and  
 131 indexed using a standard Hough transform-based automated processing at a rate of 200 points per  
 132 second. A 0.4 μm hexagonal step was applied for a scan duration of 30 minutes at each loading step.



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**Figure 2. a. Engineering stress – strain conditions at which EBSD mapping of the region of interest was performed and b. FSD map at the 970 MPa step showing slip traces and surface roughness indicative of plastic deformation**

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Operating deformation systems were first identified using a slip traces analysis at each loading step. Forward-scattered electron (FSD) micrographs are used for the slip trace detection. A FSD map of the region of interest at the 970 MPa step is shown in figure 2b. The orientation of experimental and theoretical slip traces as calculated using the EBSD data are compared.  $\{0001\}$ ,  $\{10\bar{1}0\}$  and  $\{10\bar{1}1\}$  slip planes are presently considered. Since  $\langle c+a \rangle$ -type pyramidal slip is associated with a higher slip strength than  $\langle a \rangle$ -type pyramidal slip, only  $\langle a \rangle$ -type slip was considered in the following [16-18]. A  $5^\circ$  criterion was used to assign experimental slip traces to matching basal, prismatic or pyramidal slip planes. The slip direction has to be inferred with this approach. The activated prismatic or pyramidal slip systems were directly deduced owing to the one-to-one slip direction / slip plane match. However, the basal plane is associated with three different slip directions. Prior studies reported a proper description of slip activation in Ti-6Al-4V using Schmid's law [9]. Accordingly, the basal slip system with the highest Schmid factor is assumed to be activated. Multiple – or no - matching slip planes resulted in a dismissed analysis unless all the matching systems but one exhibit very low Schmid factors ( $< 0.25$ ). Indeed, activation of a slip system with a Schmid factor lower than 0.25 is very unlikely [9,34-36]. An apparent critical resolved shear stress (CRSS) value was estimated for each successful basal or prismatic slip system identification. Assuming a global stress state, the apparent CRSS value was calculated as the product of the Schmid factor and **the average of the remote stress applied** before and after slip trace appearance. Apparent CRSS values and associated standard deviations were finally averaged over both basal and prismatic slip systems. This procedure, which relies on a homogeneous stress assumption, neglects stress heterogeneities. However, a prior study revealed that the bias introduced is limited **if a statistical approach is applied** [37].

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In order to study lattice rotations at the nodule / colony scale, pre-processing of the raw crystallographic orientation data was performed using OIM analysis software. The following steps are applied. (i) Data points with a confidence index below 0.1 were dismissed in order to rule out unreliable data points. (ii) Separate nodules / colonies were identified using a  $2^\circ$  misorientation criterion. (iii) The average crystallographic orientations of the 34 nodules and the 21 colonies considered in the present study were computed. The resulting Euler angles  $(\varphi_1, \Phi, \varphi_2)$  were then processed using an in-house Matlab code in order to calculate the lattice rotation relative to the

166 initial lattice orientation. The crystalline orientation at step  $i$  is expressed in the specimen frame  
 167 using the rotation matrix  $\mathbf{R}_{0,i}$  defined as follows (3).

$$168 \quad \mathbf{R}_{0,i} =$$

$$169 \quad \begin{bmatrix} \cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi & -\sin \varphi_2 \cos \varphi_1 - \cos \varphi_2 \sin \varphi_1 \cos \Phi & \sin \varphi_1 \sin \Phi \\ \cos \varphi_2 \sin \varphi_1 + \sin \varphi_2 \cos \varphi_1 \cos \Phi & -\sin \varphi_1 \sin \varphi_2 + \cos \varphi_1 \cos \varphi_2 \cos \Phi & -\cos \varphi_1 \sin \Phi \\ \sin \varphi_2 \sin \Phi & \cos \varphi_2 \sin \Phi & \cos \Phi \end{bmatrix}$$

$$170 \quad (3)$$

171 The lattice rotation between step  $j$  and step  $i$  is described using the rotation matrix  $\Delta \mathbf{R}_{i,j}$  given in  
 172 equation (4).

$$173 \quad \Delta \mathbf{R}_{i,j} = \mathbf{R}_{0,j} \mathbf{R}_{0,i}^{-1} \quad (4)$$

174 The magnitude of the rotation, which is denoted as  $\theta_{i,j}$ , is computed using equation (5).

$$175 \quad \theta_{i,j} = \cos^{-1} \left( \frac{\Delta R_{i,j 11} + \Delta R_{i,j 22} + \Delta R_{i,j 33} - 1}{2} \right) \quad (5)$$

176 Single slip in a constrained crystal is accompanied by lattice rotation. According to equation  
 177 (2), the associated rotation axis under single slip condition is normal to both the slip plane normal  
 178 and the slip direction. This axis is denoted in the following as the slip-induced rotation axis. The slip  
 179 plane normals  $\vec{n}_{i,s}$  and the slip directions  $\vec{m}_{i,s}$  are expressed in the specimen frame for the slip  
 180 system  $s$  at each loading step  $i$  according to equations (6) and (7).

$$181 \quad \vec{n}_{i,s} = \mathbf{R}_{0,i} \cdot \vec{n}_{0,s} \quad (6)$$

$$182 \quad \vec{m}_{i,s} = \mathbf{R}_{0,i} \cdot \vec{m}_{0,s} \quad (7)$$

183 The normal to both slip plane normal and slip direction (i.e. the slip induced rotation axis) for  
 184 each slip system is then calculated using equation (8).

$$185 \quad \vec{t}_{i,s} = \vec{n}_{i,s} \wedge \vec{m}_{i,s} \quad (8)$$

186 Prior works reported that  $\langle a \rangle$  or  $\langle c+a \rangle$  pyramidal slip is associated with rare observations  
 187 [9,10]. In the present work, only basal and prismatic slip systems are considered in order to simply  
 188 the prediction of operating slip systems owing to a reduced number of potential slip induced rotation  
 189 axes. Each basal slip system leads to a distinct rotation axis whereas prismatic slip is associated with a  
 190 single rotation axis for any considered slip system. The magnitude of the rotation between loading  
 191 steps  $i$  and  $j$  was computed for the 4 slip induced rotation axis. Assuming a negligible rigid body  
 192 rotation of the grain, the magnitude of the rotation should be the lowest for the operating slip  
 193 system.

194 The angle of the rotation from  $\vec{t}_{i,s}$  to  $\vec{t}_{j,s}$ , which is denoted as  $\alpha_{i,j,s}$ , is calculated for each slip  
 195 system  $s$  using equation (9).

$$196 \quad \alpha_{i,j,s} = \cos^{-1}(\langle \vec{t}_{i,s}, \vec{t}_{j,s} \rangle) \quad (9)$$

197 This approach implicitly implies that only single slip can be properly considered. Hence, the  
 198 tensile test was stopped after 3% total strain in order to avoid frequent multiple slip occurrences.  
 199 Similarly, cross-slip may also induce deviations of the theoretical slip induced rotation axis. This latter  
 200 point can be dismissed in the present conditions since cross-slip is inhibited in titanium alloys with a  
 201 high aluminum content owing to planar slip [8].

202 A reliable prediction of the operating slip system also requires an accurate determination of  
 203 the slip induced rotation axis. However, a prior study based on individual orientation measurement  
 204 using EBSD reported that the misorientation axis is essentially undetermined for an applied rotation  
 205 of 5°, or less. In the present work, instead of using individual measurements, the measurements are  
 206 averaged over more than 500 points. Compared to single measurements, the resulting orientation  
 207 has a significantly improved precision. The standard deviation of the average orientation  $std(\bar{\theta})$  is  
 208 given below as a function of  $std(\theta)$  the standard deviation of individual measurements and  $N$  the  
 209 number of measurements used for the average.

$$210 \quad std(\bar{\theta}) = \frac{std(\theta)}{\sqrt{N}} \quad (10)$$

211 The standard deviation in the orientation calculation is then reduced by a factor higher than  
 212 20. A correct prediction of the slip induced rotation axis is demonstrated in Appendix 1 for rotation  
 213 magnitudes as low as 0.1°. However, other effects, such as rigid –body rotations or free surface  
 214 related effects, could influence the results. This is discussed in the following sections.

215 The slip induced rotation axis being widely employed in the following, it is referred to as SIR  
 216 axis. In addition, the angle of rotation being systematically discussed relatively to the initial  
 217 orientation, it is simply denoted as angle of rotation.

218

### 219 3. Results

#### 220 3.1 Slip trace analysis

221 Slip traces were observed on the surface of 32 nodules among 34 nodules considered. A slip  
 222 traces analysis was performed in order to identify the activated slip systems in these nodules. The  
 223 applied stress at which the slip trace was detected, the operating slip mode and the apparent CRSS  
 224 are reported in table 1 for each nodule. The first basal slip trace was observed at the 785 MPa step  
 225 while the first prismatic slip band was observed at the 840 MPa step. According to this observation,  
 226 the activation of basal slip proceeds at a lower macroscopic stress magnitude than the activation of  
 227 prismatic slip. The same activation kinetics have been reported for Ti-6Al-4V and other titanium  
 228 alloys with similar aluminum contents [10-12]. **Observations of pyramidal slip are occasional (3**  
 229 **occurrences out of 34 nodules).** Hence, this slip system can reasonably be excluded from the analysis  
 230 of deformation processes using lattice rotations. The average apparent CRSS is about 364 MPa for  
 231 basal slip versus about 375 MPa for prismatic slip. These values are consistent with estimates  
 232 reported in prior studies [36]. The basal / prismatic CRSS ratio is about 0.97 which is also in good  
 233 agreement with previous results. The standard deviations of basal and prismatic CRSS values are 55  
 234 MPa and 37 MPa respectively. Standard deviations extracted from prior studies focusing on similar  
 235 titanium alloys are in the 20 MPa – 40 MPa range [10-12,37]. The present values are thus slightly  
 236 higher than the ones previously reported. This observation is most likely related to the rough  
 237 description of slip activation kinetics. Indeed, a low number of stops was performed in the stress  
 238 range below the 0.2 % proof stress, in which a gradual activation of basal and prismatic slip systems  
 239 is observed [10]. Slip traces analysis is usually based on secondary electron micrographs or back-  
 240 scattered electron micrographs. Interestingly, consistent results were obtained using FSD  
 241 micrographs, which were taken on a 70° tilted specimen.

| Nodule N° | Applied stress at slip trace detection (MPa) | Activated slip system according to slip trace analysis | Apparent CRSS | Remark |
|-----------|--|--|---------------|--------|
| Nodule 1  | 785  | Basal  | 361.1         |        |



|           |     |           |       |  |
|-----------|-----|-----------|-------|--|
| Nodule 2  | 900 | Basal     | 232.6 |  |
| Nodule 3  | 840 | Pyramidal | 333.9 |  |
| Nodule 4  | 875 | Basal     | 436.8 |  |
| Nodule 5  | 840 | Basal     | 394.4 |  |
| Nodule 6  | 785 | Basal     | 378.8 |  |
| Nodule 7  | 935 | Prismatic | 283.7 |  |
| Nodule 8  | 920 |           |       | Unidentified - No matching slip trace                                    |
| Nodule 9  | 920 | Basal     | 266.8 |  |
| Nodule 10 | 840 | Basal     | 373.5 |  |
| Nodule 11 | 840 | Basal     | 364.5 |  |
| Nodule 12 | 875 | Prismatic | 363.1 |  |
| Nodule 13 | 875 |           |       | Unidentified - Multiple matching slip traces with high Schmid factors    |
| Nodule 14 | 785 | Basal     | 363.3 |  |
| Nodule 15 | 840 | Prismatic | 394.0 |  |
| Nodule 16 | 840 | Basal     | 403.6 |  |
| Nodule 17 |     |           |       | No slip trace detected   |
| Nodule 18 | 900 | Pyramidal | 421.5 |  |
| Nodule 19 | 920 | Basal     | 426.5 |  |
| Nodule 20 | 785 | Basal     | 378.7 | Multiple matching slip traces with low Schmid factors (< 0.25)           |
| Nodule 21 | 935 | Prismatic | 376.2 |  |
| Nodule 22 | 900 |           |       | Unidentified - Multiple matching slip traces with high Schmid factors    |
| Nodule 23 | 840 | Basal     | 370.9 |  |
| Nodule 24 | 900 | Prismatic | 430.1 |  |
| Nodule 25 | 900 | Prismatic | 402.1 |  |
| Nodule 26 | 920 | Prismatic | 343.0 |  |
| Nodule 27 |     |           |       | No slip trace detected   |
| Nodule 28 | 840 | Pyramidal | 314.7 |  |
| Nodule 29 | 900 | Prismatic | 371.6 |  |
| Nodule 30 | 875 | Prismatic | 376.3 |  |
| Nodule 31 | 785 | Basal     | 345.2 |  |
| Nodule 32 | 920 | Prismatic | 356.1 |  |
| Nodule 33 | 875 | Prismatic | 397.6 | Other matching slip trace: pyramidal slip with low Schmid factor (<0.25) |
| Nodule 34 | 875 | Prismatic | 400.7 |  |

242 **Table 1. Nodule number, applied stress at which slip traces were first detected, activated slip mode**  
243 **according to the slip trace analysis, apparent CRSS (determined using a global stress state) and**  
244 **supplementary remark for the 34 nodules considered**

245 *3.2 Prediction of activated slip systems using lattice rotation data*

246 Deformation systems operating in nodules were then studied regarding lattice rotation data.  
247 According to the FSD micrographs, no slip activity was observed up to 750 MPa. Since only slip-  
248 induced rotation is used for the identification of operating slip systems, the angle of rotation of slip-  
249 induced rotation axes for basal and prismatic slip systems were calculated between the 750 MPa step  
250 and the 970 MPa step. This enables to limit the contribution of elastic deformation to the rotation of  
251 the slip-induced rotation axes while considering substantial rotation magnitudes. The results and the  
252 associated Schmid factors are presented in table 2. Since only one slip-induced rotation axis is  
253 associated with prismatic slip systems, only the highest Schmid factor is reported. A few nodules (2,  
254 7, 31) have been ruled out of the present analysis as crystal symmetries induced artificially large  
255 magnitudes of rotations (highlighted in grey in Table 2). For each nodule, the slip system with the  
256 lowest angle was predicted as activated (highlighted in green in table 2). The ratio of the associated  
257 Schmid factor to the maximum Schmid factor among basal and prismatic slip systems and the  
258 agreement with the operating slip mode identified according to the slip trace analysis are also  
259 indicated.

| Nodule N° | Basal 1 Schmid factor | Basal 1 rotation (°) | Basal 2 Schmid factor | Basal 2 rotation (°) | Basal 3 Schmid factor | Basal 3 rotation (°) | Maximum prismatic Schmid factor | Prismatic rotation (°) | Predicted slip system | Predicted SF / Maximum SF | Agreement with slip traces analysis |
|-----------|-----------------------|----------------------|-----------------------|----------------------|-----------------------|----------------------|---------------------------------|------------------------|-----------------------|---------------------------|-------------------------------------|
| Nodule 1  | 0.388                 | 0.689                | 0.072                 | 1.089                | 0.460                 | 0.385                | 0.208                           | 1.090                  | B3                    | 1.000                     | True                                |
| Nodule 2  | 0.258                 | 59.584               | 0.220                 | 59.584               | 0.038                 | 59.584               | 0.041                           | 0.288                  |                       |                           |                                     |
| Nodule 3  | 0.417                 | 0.632                | 0.085                 | 0.837                | 0.332                 | 0.263                | 0.365                           | 0.879                  | B3                    | 0.797                     | -                                   |
| Nodule 4  | 0.499                 | 0.000                | 0.262                 | 1.573                | 0.237                 | 1.552                | 0.213                           | 1.817                  | B1                    | 1.000                     | True                                |
| Nodule 5  | 0.156                 | 0.826                | 0.313                 | 0.354                | 0.470                 | 0.723                | 0.320                           | 0.808                  | B2                    | 0.667                     | True                                |
| Nodule 6  | 0.483                 | 0.445                | 0.239                 | 1.241                | 0.244                 | 1.079                | 0.161                           | 1.217                  | B1                    | 1.000                     | True                                |
| Nodule 7  | 0.356                 | 60.402               | 0.217                 | 60.402               | 0.139                 | 60.402               | 0.408                           | 0.288                  |                       |                           |                                     |
| Nodule 8  | 0.410                 | 0.807                | 0.184                 | 1.275                | 0.226                 | 0.824                | 0.361                           | 1.101                  | B1                    | 1.000                     | -                                   |
| Nodule 9  | 0.290                 | 0.632                | 0.014                 | 0.596                | 0.276                 | 0.641                | 0.055                           | 0.352                  | P                     | 0.191                     | -                                   |
| Nodule 10 | 0.391                 | 1.034                | 0.054                 | 1.599                | 0.445                 | 1.478                | 0.296                           | 1.351                  | B1                    | 0.879                     | True                                |
| Nodule 11 | 0.413                 | 0.866                | 0.434                 | 0.385                | 0.021                 | 1.122                | 0.272                           | 1.141                  | B2                    | 1.000                     | True                                |
| Nodule 12 | 0.242                 | 0.449                | 0.011                 | 0.264                | 0.231                 | 0.274                | 0.414                           | 0.368                  | B2                    | 0.026                     | False                               |
| Nodule 13 | 0.366                 | 0.161                | 0.085                 | 1.518                | 0.451                 | 1.454                | 0.317                           | 1.683                  | B1                    | 0.812                     | -                                   |
| Nodule 14 | 0.463                 | 0.677                | 0.105                 | 0.983                | 0.358                 | 0.838                | 0.189                           | 0.820                  | B1                    | 1.000                     | True                                |
| Nodule 15 | 0.112                 | 0.514                | 0.016                 | 0.709                | 0.128                 | 0.571                | 0.469                           | 0.451                  | P                     | 1.000                     | True                                |
| Nodule 16 | 0.481                 | 0.650                | 0.191                 | 1.601                | 0.289                 | 2.227                | 0.180                           | 2.309                  | B1                    | 1.000                     | True                                |
| Nodule 17 | 0.460                 | 0.258                | 0.064                 | 1.187                | 0.396                 | 1.199                | 0.219                           | 1.347                  | B1                    | 1.000                     | -                                   |
| Nodule 18 | 0.383                 | 0.769                | 0.137                 | 0.765                | 0.246                 | 0.744                | 0.399                           | 0.349                  | P                     | 1.000                     | -                                   |
| Nodule 19 | 0.462                 | 0.261                | 0.372                 | 0.873                | 0.090                 | 1.047                | 0.296                           | 1.118                  | B1                    | 1.000                     | True                                |
| Nodule 20 | 0.482                 | 0.495                | 0.147                 | 0.748                | 0.335                 | 0.810                | 0.212                           | 0.699                  | B1                    | 1.000                     | True                                |
| Nodule 21 | 0.379                 | 0.000                | 0.244                 | 0.630                | 0.135                 | 0.606                | 0.402                           | 0.708                  | B1                    | 0.943                     | False                               |
| Nodule 22 | 0.148                 | 0.075                | 0.064                 | 0.197                | 0.212                 | 0.134                | 0.474                           | 0.212                  | B1                    | 0.313                     | -                                   |
| Nodule 23 | 0.442                 | 0.437                | 0.135                 | 0.934                | 0.307                 | 0.986                | 0.143                           | 1.008                  | B1                    | 1.000                     | True                                |
| Nodule 24 | 0.198                 | 0.481                | 0.056                 | 0.667                | 0.142                 | 0.682                | 0.478                           | 0.557                  | B1                    | 0.414                     | False                               |
| Nodule 25 | 0.197                 | 0.479                | 0.027                 | 0.432                | 0.224                 | 0.385                | 0.447                           | 0.265                  | P                     | 1.000                     | True                                |
| Nodule    | 0.419                 | 0.461                | 0.107                 | 0.464                | 0.312                 | 0.577                | 0.372                           | 0.453                  | P                     | 0.888                     | True                                |

|           |       |        |       |        |       |        |       |       |    |       |       |
|-----------|-------|--------|-------|--------|-------|--------|-------|-------|----|-------|-------|
| 26        |       |        |       |        |       |        |       |       |    |       |       |
| Nodule 27 | 0.476 | 0.026  | 0.132 | 0.651  | 0.345 | 0.661  | 0.295 | 0.732 | B1 | 1.000 | -     |
| Nodule 28 | 0.053 | 0.990  | 0.039 | 0.964  | 0.092 | 0.965  | 0.467 | 0.188 | P  | 1.000 | -     |
| Nodule 29 | 0.218 | 0.642  | 0.004 | 0.562  | 0.214 | 0.548  | 0.411 | 0.411 | P  | 1.000 | True  |
| Nodule 30 | 0.030 | 0.345  | 0.015 | 0.283  | 0.015 | 0.386  | 0.436 | 0.256 | P  | 1.000 | True  |
| Nodule 31 | 0.027 | 60.043 | 0.440 | 60.040 | 0.412 | 60.038 | 0.190 | 0.796 |    |       |       |
| Nodule 32 | 0.238 | 0.833  | 0.127 | 0.500  | 0.111 | 0.718  | 0.425 | 0.776 | B2 | 0.300 | False |
| Nodule 33 | 0.234 | 0.750  | 0.090 | 0.790  | 0.144 | 0.814  | 0.454 | 0.418 | P  | 1.000 | True  |
| Nodule 34 | 0.019 | 0.733  | 0.009 | 0.751  | 0.011 | 0.710  | 0.458 | 0.258 | P  | 1.000 | True  |

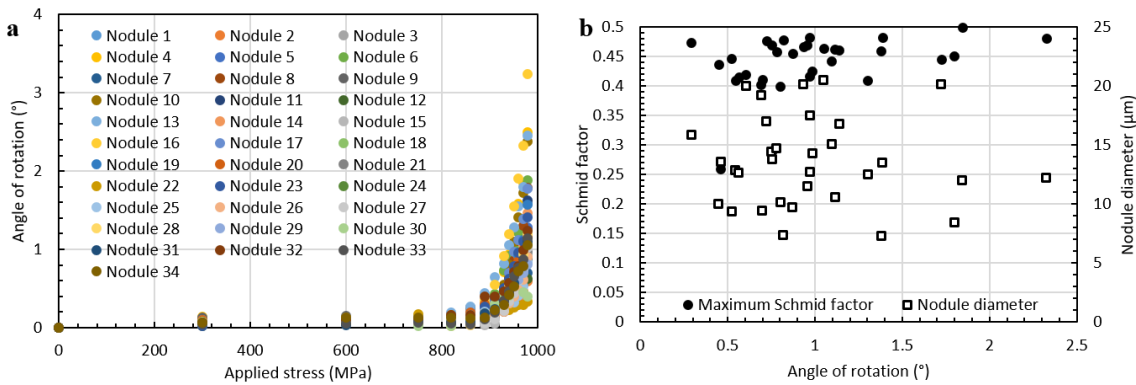
260 **Table 2. Nodule number, Schmid factors and angle of rotation of slip-induced rotation axes between 750**  
261 **MPa and 970 MPa for basal and prismatic slip systems. The predicted slip system is highlighted in green. The**  
262 **ratio of its Schmid factor to the maximum Schmid factor and the agreement with slip traces analysis are also**  
263 **indicated.**

264 The ratio of the Schmid factor associated with the slip system predicted as activated to the  
265 maximum Schmid factor among basal and prismatic slip systems is reported in table 2. In most cases,  
266 the slip system which was predicted as activated using lattice rotations is the slip system with the  
267 highest Schmid Factor among the basal and prismatic slip systems. This is confirmed by the  
268 magnitude of the ratio, which is about 0.85 on average. According to the data presented in table 2,  
269 the Schmid factor of the slip systems predicted as activated is about 0.38 on average. The Schmid  
270 factor being a well-established indicator of slip activation likeliness in titanium alloys [9], this value  
271 points out a consistent prediction of activated slip systems using lattice rotations.

272 A comparison with the results obtained using the slip trace analysis was also carried out. The  
273 agreement between the active slip mode predicted using lattice rotations and the active slip mode  
274 identified according to the slip trace analysis is indicated in table 2. Since pyramidal slip systems have  
275 not been considered for the identification of active slip system using lattice rotations, only nodules  
276 exhibiting basal or prismatic slip traces are considered. A very good agreement is found with an 82 %  
277 success rate of prediction. As a comparison, this value is typical of a slip trace analysis [10]. A  
278 disagreement between both approaches was found for nodules 12, 21, 24 and 32. Several potential  
279 causes have been identified. To begin with, the slip system prediction relies on a single slip  
280 assumption. A careful observation of the slip traces shown in figure 2b suggests that most grains  
281 seem deformed by single slip at 970 MPa. Only 4 out of the 34 nodules present slip traces suggesting  
282 an activity of several slip systems (nodules 2, 3, 10 and 30). However, no relation could be found with  
283 incorrect predictions. This may suggest that the slip system which is activated first dominates the  
284 lattice rotation behavior in the present conditions. A low rotation magnitude may also be an  
285 influential parameter. For instance, the angles of rotation associated with the slip-induced rotation  
286 axes of nodule 12, which is associated with an erroneous prediction, are very small ( $< 0.45^\circ$ ) and  
287 contained a restricted interval. These characteristics renders the analysis highly sensitive to rigid-  
288 body rotation, such as induced by surrounding grains.

289 The slip trace analysis was presently considered as a reference procedure. However, an  
 290 inherent bias is introduced. Hence, some predictions might be wrongly considered as ‘incorrect’. For  
 291 instance, a high Schmid factor is found for the slip system predicted as activated in nodule 21 using  
 292 lattice rotations. The corresponding slip direction has a low component magnitude in the direction  
 293 normal to the specimen surface (18 % of the total magnitude). The associated slip traces may have  
 294 been missed due to insufficiently high slip steps that caused the poor agreement between both  
 295 active slip system identification techniques. This points out a major advantage of a lattice rotation  
 296 based slip system identification: even slip leading to very small slip steps can be detected. In  
 297 addition, a major drawback of slip traces based procedures is that the identification only relies on slip  
 298 planes while slip directions are inferred. As a consequence, basal slip traces are often assumed as  
 299 associated with the basal slip system with the highest Schmid factor [9,10,35,38]. The ratio of the  
 300 basal Schmid factor identified using lattice rotations to the maximum basal Schmid factor was  
 301 computed for successful basal slip predictions. The average value, which is about 0.96, is very close  
 302 to 1. Hence, the aforementioned assumption, which is often used without verification, seems  
 303 actually reasonable.

### 304 3.3 Lattice rotation in nodules

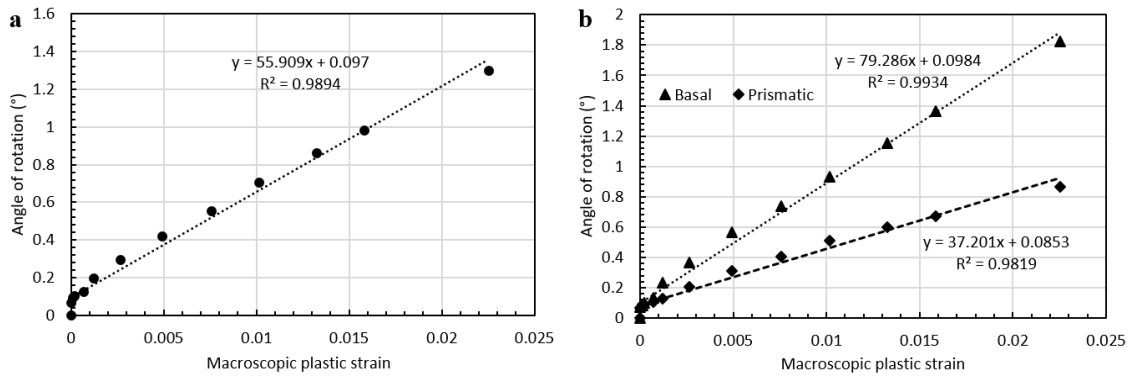


305  
 306 **Figure 3 a. Average angle of rotation of each nodule, which is plotted against the applied stress, showing a**  
 307 **sharp increase in magnitude at the onset of plastic slip and b. Schmid factor and nodule diameter plotted**  
 308 **against the average angle of rotation of each nodule at the 970 MPa step**

309 Lattice rotation relative to the initial orientation was calculated at each loading step using  
 310 equation (5). The angle of rotation is plotted against the applied stress in figure 3 a for each nodule.  
 311 In the elastic regime, i.e. for an applied stress below 820 MPa, the angles of rotation remain below  
 312 0.2 °. A subtle and progressive increase of the average value was noticed from 0.065 ° at 300 MPa to  
 313 0.094 ° at 750 MPa. A marked increase in the angle of rotation is coincident with the onset of slip  
 314 activity, i.e. for an applied stress higher than 750 MPa according to the slip trace analysis. At 978  
 315 MPa, the nodule with the highest magnitude of rotation experienced a 3.3° rotation while the nodule  
 316 with the lowest magnitude of rotation experienced a 0.4° rotation. The magnitude of the rotations in  
 317 the elastic regime are thus small compared to the magnitude of the rotations associated with roughly  
 318 2 % plastic strain. In addition, the spread of the values obtained at 978 MPa testifies of a highly  
 319 heterogeneous rotation behavior in the plastic regime.

320 In order to identify factors potentially accounting for such dispersion, the influence of several  
 321 parameters was examined. The effect of the nodule size was investigated first. **Indeed, the grain size**  
 322 **is highly influent on deformation owing to a high strength associated with low grain sizes [39,40].** The  
 323 diameter of each nodule is plotted with respect to the angle of rotation at 970 MPa in figure 3 b. No  
 324 marked effect of the nodule size could be found in the present conditions. Multiple prior studies  
 325 showed that the Schmid factor is highly correlated with slip activity in titanium alloys. The influence

326 of this parameter on the rotation magnitude was then investigated. The maximum Schmid factor  
 327 among basal and prismatic slip systems for each nodule was plotted with respect to the angle of  
 328 rotation at 970 MPa in figure 3 b. The nodules with a high angle of rotation exhibit high maximum  
 329 Schmid factors while nodules with a low maximum Schmid factor are associated with low angles of  
 330 rotation. Notwithstanding, nodules with a high maximum Schmid factor also occasionally exhibit low  
 331 angles of rotation. Thus, these parameters seem insufficient to fully account for the dispersions  
 332 previously highlighted.



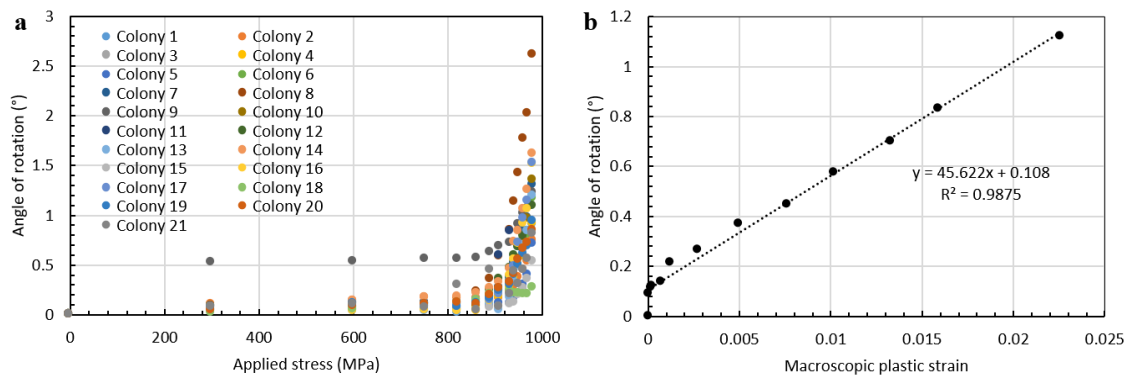
333

334 **Figure 4 a. Average angle of rotation over the 34 nodules showing a linear dependence with respect to**  
 335 **macroscopic plastic strain, b. Angle of rotation averaged over nodules exhibiting basal or prismatic slip**  
 336 **activity and plotted against macroscopic plastic strain. Significantly different rotation behaviors are**  
 337 **evidenced.**

338 The angle of lattice rotation relative to the initial orientation was then averaged over the 34  
 339 nodules considered and plotted against the macroscopic plastic strain in figure 4 a. An offset about  
 340 0.1 ° is observed at the end of the elastic regime. Beyond, the average angle of rotation increases  
 341 linearly with respect to the macroscopic plastic strain. A 56° slope is obtained using a linear  
 342 regression. The value of the regression coefficient, which is about 0.989, indicates a very good fit to  
 343 the experimental data. This result confirms the direct relationship between the plastic strain  
 344 magnitude and the magnitude of lattice rotations. In the following, the set of nodules is split into  
 345 subsets in order to probe the effect of the operating slip mode on the lattice rotation behavior as  
 346 well as the related plastic strain partitioning.

347 A potential difference in the lattice rotation behavior of nodules with operating basal or  
 348 prismatic slip systems was first investigated. In order to retain solely nodules with confidently  
 349 identified slip systems, only nodules with a similar slip mode predicted using slip traces analysis and  
 350 lattice rotations were considered. 11 nodules are contained in the subset corresponding to basal slip  
 351 while 7 nodules are contained in the subset corresponding to prismatic slip. The angles of rotation  
 352 relative to the initial orientation were averaged over each subset of nodules. The resulting values are  
 353 plotted against the macroscopic plastic strain in figure 4 b. For each subset, a linear relationship  
 354 between the average angle of rotation and the plastic strain magnitude is noticed. Linear regressions  
 355 are associated with coefficients higher than 0.98. These values indicate very good fits to the  
 356 experimental data. The slope is about 79 ° for the subset associated with basal slip while the slope is  
 357 about 37 ° for the subset associated with prismatic slip. This significant difference highlights a strong  
 358 dependence of the lattice rotation behavior on the operating slip mode.

### 359 3.4 Lattice rotation in colonies



360

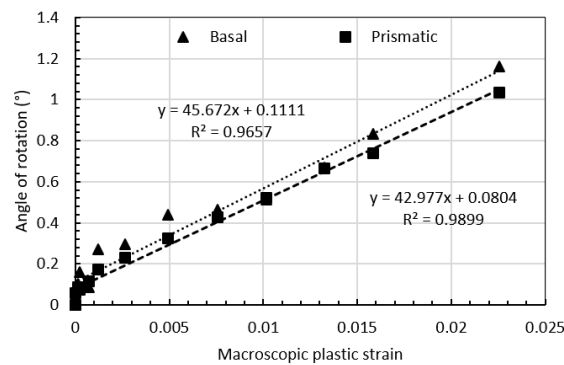
361 **Figure 5 a. Average angle of rotation of each colony, which is plotted against the macroscopic plastic strain,**  
 362 **showing a sharp increase in magnitude at the onset of plastic slip and b. Angle of rotation averaged over the**  
 363 **21 colonies and plotted against the macroscopic plastic strain. A linear dependence with respect to the**  
 364 **macroscopic plastic strain is noticed. The magnitude of the slope is lower than the one obtained for nodules.**

365 According to prior studies, nodules and colonies exhibit different deformation behaviors. As a  
 366 consequence, a potential difference in the lattice rotation behaviors was investigated. 3 colonies  
 367 were ruled out of the present analysis as crystal symmetries induced artificially large magnitude of  
 368 rotations. The angle of rotation relative to the initial orientation is plotted against the applied stress  
 369 in figure 5 a. The same qualitative trends as for nodules are observed. In average, the angle of  
 370 rotation is low for a macroscopic applied stress lower than 820 MPa. A sudden increase in the angle  
 371 of rotation is coincident with the onset of macroscopic yield. In order to quantitatively assess the  
 372 average lattice rotation behavior in colonies, the angle of rotation relative to the initial orientation  
 373 was averaged at each step over the 18 colonies considered. The resulting values are plotted against  
 374 the macroscopic plastic strain in figure 5 b. The average angle of rotation increases linearly with  
 375 respect to the macroscopic plastic strain. As a consequence, a linear regression was applied to enable  
 376 a quantified comparison with the lattice rotation behavior of nodules. According to the regression  
 377 coefficient ( $\approx 0.988$ ), a very good fit to the data is obtained with a 46 ° slope. This value is lower than  
 378 the one previously established considering nodules only. Hence, the rotation of colonies appears  
 379 more difficult than the rotation of nodules for a given macroscopic plastic strain increment.  
 380 Concurrently, the average angle of rotation is lower for colonies than for nodules considering a  
 381 similar macroscopic plastic strain. For instance, under an applied stress of 970 MPa, the average  
 382 angle of rotation is about 0.82 ° for colonies versus 0.98 ° for nodules. The origins of these  
 383 differences are discussed in the next section.

384 Finally, a potential difference in the lattice rotation behavior of colonies with operating basal  
 385 or prismatic slip systems was investigated. A slip trace analysis was carried out in order to identify  
 386 the operating slip systems. Among the 21 colonies considered, slip traces were confidently assigned  
 387 to a prismatic slip system for 7 colonies and to a basal slip system for 4 colonies. An operating slip  
 388 mode could not be identified for 10 colonies. Slip traces were either absent or not confidently  
 389 assigned to a basal or prismatic slip system. The restricted number of cases presently considered  
 390 ruled out any reliable apparent CRSS estimation.

391 At each step, the angle of rotation relative to the initial orientation was averaged over  
 392 colonies with a similar operating slip mode. The resulting values are plotted against the macroscopic  
 393 plastic strain in figure 6. The average angles of rotation associated with the operation of basal slip are  
 394 slightly higher than the average angles of rotation associated with the operation of prismatic slip. For  
 395 instance, under an applied stress of 970 MPa, the angles are 0.75 ° for prismatic slip and 0.82 ° for  
 396 basal slip. A linear regression was applied to both datasets. Regression coefficients about 0.966 and

397 0.990 were obtained for basal and prismatic slip respectively. These values, which are very close to 1,  
 398 indicate a good fit to the data. A slope of 46 ° was obtained for the subset of colonies associated with  
 399 the operation of basal slip while a slope of 43 ° was obtained for the subset of colonies associated  
 400 with the operation of prismatic slip. As with nodules, the subset associated with basal slip exhibits a  
 401 higher slope than the subset associated with prismatic slip. However, the difference in the slope  
 402 values is substantially decreased. Using the slope of the subset associated with the operation of basal  
 403 slip as a reference, the slope corresponding to the subset associated with the operation of prismatic  
 404 slip is 53 % lower for nodules while only 6 % lower for colonies. Hence, the differences in the lattice  
 405 rotation behavior between basal and prismatic slip modes seem mitigated if colonies are considered.  
 406 Owing to the limited number of colonies presently considered, the previous analysis was repeated in  
 407 a neighboring region. The data, which are not shown here for clarity purposes, support the previous  
 408 findings.



409

410 **Figure 6. Angle of rotation averaged over colonies exhibiting basal or prismatic slip activity and plotted**  
 411 **against macroscopic plastic strain**

412 **4. Discussion**

413 *4.1 Identification of deformation processes using lattice rotations*

414 Local lattice rotations were characterized up to about 2 % plastic strain using an in situ EBSD  
 415 tensile test. Based on this data, the identification of active deformation systems was undertaken. A  
 416 good agreement was found with a slip trace analysis, which is a more conventional procedure. The  
 417 following conclusions ensue: i) the rigid body rotations resulting from processes such as specimen  
 418 realignment under loading or grain shape rotations induced by neighboring grains appear as having a  
 419 minor contribution to the measured lattice rotations, even if a single grain is considered. ii) In  
 420 contrast, intragranular plastic slip has a dominant contribution to the measured lattice rotations.  
 421 Interestingly, the occasional operation of two slip systems in a single nodule did not disrupt the  
 422 analysis, which is based on a single slip assumption. This observation may suggest that the first slip  
 423 system to be activated dominates the slip-induced lattice rotation.

424 The main advantage offered by the lattice rotation based procedure is the discrimination of  
 425 slip systems sharing the same slip plane. For instance, basal slip systems could be differentiated  
 426 regarding slip directions. In contrast, slip trace analysis usually relies on strong assumptions to  
 427 identify the active slip system since the slip trace only reflects the slip plane. Basal slip traces are  
 428 often assumed to correspond to the basal slip system with the highest Schmid factor [9,10,36]. The  
 429 present lattice rotation based analysis showed that this hypothesis is actually consistent with  
 430 experimental observations. However, some limitations, which are discussed hereafter, are inherent  
 431 to the method.

432 Despite the promising results obtained, occasional misidentification of slip systems are  
433 suspected. Criteria and confidence indices have yet to be introduced in order to obtain a robust  
434 analysis of deformation systems. Although further work is required in this direction, several  
435 parameters can be readily identified as affecting the reliability of the prediction. The operating slip  
436 system being identified according to the angle of rotation of slip induced rotation axes, predictions  
437 should be given credit provided the magnitude of lattice rotations are higher than a given angular  
438 threshold. This threshold is partly related to the repeatability of orientation measurements. Such  
439 values are lower than the classical value of 0.5 ° for EBSD angular resolution owing to the averaging  
440 approach presently applied [41]. As shown in Appendix I, the scatter in the data is small, with the  
441 rotation from one measured orientation to another being on average 0.02°, and at most 0.05°. In  
442 turn, this enabled an improved determination of the rotation axis for small rotation angles compared  
443 to single orientation measurements. The reader is referred to Appendix I for further details. Since the  
444 orientations used in the present analyses result from averaging over hundreds of single orientation  
445 measurements carried out in a single grain, the number of orientation measurements performed  
446 inside a single grain is also a parameter that has to be considered. Besides, any assessment of slip  
447 activation kinetics is still a challenge due to a difficult detection of slip activation. Improved precision  
448 could be attained using optimized EBSD acquisition settings [42], improved Kikuchi patterns indexing  
449 techniques [43] or cross-correlation based high angular resolution EBSD [41].

450 Some erroneous identifications of slip systems may also be ascribed to the influence of rigid-  
451 body rotations. For instance, these rotations are the result of the loading conditions of the specimen,  
452 which cannot allow a perfect alignment of the specimen with the EBSD frame during the whole  
453 duration of the tensile test, and the presence of the free surface, which implies an incomplete  
454 constraint of nodules and colonies. As a consequence, the measured rotation axis may somewhat  
455 deviate from the expected one. The contribution related to rigid body rotations may thus be  
456 noticeable if small angles of rotation are involved. Finally, the number of potential slip systems,  
457 which is tightly related to the number of slip induced rotation axes, controls the complexity of the  
458 lattice rotation behavior. The higher the number of potential slip systems is, the more subtle the  
459 discrimination between the angles of rotation of the slip induced rotation axes is. This is another  
460 limitation of this procedure.

#### 461 4.2 Towards a quantitative assessment of plastic strain?

462 In situ characterization of lattice rotations during tensile deformation highlighted a linear  
463 relation between the average angle of lattice rotation relative to the initial orientation and the  
464 macroscopic plastic strain. Such a correlation is consistent with data reported in prior studies  
465 focusing on X-ray diffraction characterization of lattice rotations in 316 stainless steel [29] and in  
466 commercial purity titanium [32]. The crystal plasticity models involving equation (2) can also predict  
467 this feature provided the following conditions are met: i) single slip conditions, ii) a negligible  
468 influence of rigid-body spins and iii) a limited evolution of the skew-symmetric Schmid tensor with  
469 deformation (i.e. of the crystallographic orientations). These conditions being satisfied in the present  
470 work, lattice rotations measured using in situ EBSD can be used to assess strain partitioning in Ti-6Al-  
471 4V. The relation between the lattice rotation and the plastic strain is discussed in the following.

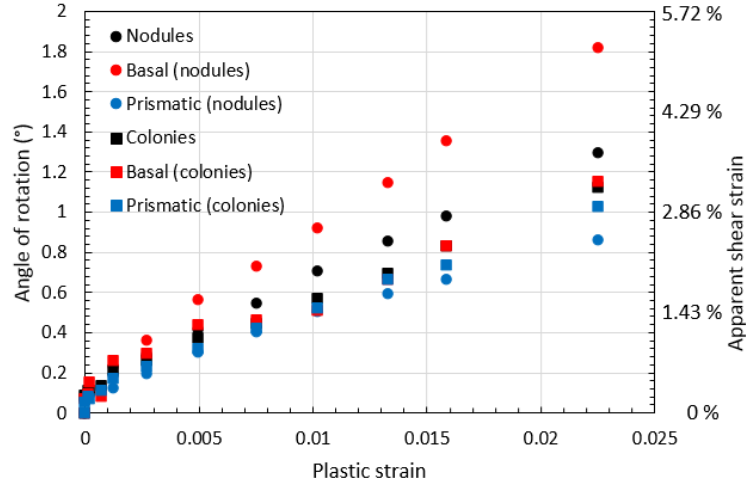
472 Equation (2) leads to a direct relationship between the plastic shear rate  $\dot{\gamma}$  and the lattice  
473 rotation rate  $W^*$ . Equation (7), which is defined below, can be used for time integration [33].

$$474 \mathbf{R}_{0,j} = \mathbf{R}_{0,i} \exp(\mathbf{W}^* \Delta t) \quad (7)$$

475 The relationship between the shear on the active slip system and the magnitude of lattice  
476 rotation is straightforward. A linear relation with a slope about 28.6 ° is analytically predicted.



477 Accordingly, the measured angles of lattice rotation can be converted into apparent plastic shear  
 478 strain magnitudes. The average angles of rotation previously obtained were converted into apparent  
 479 plastic shear strain and plotted in figure 7 against the macroscopic plastic strain. The apparent shear  
 480 strain magnitudes are discussed in the following subsection (4.3) regarding microstructural features  
 481 and active slip modes.



482

483 **Figure 7: Average angle of rotation and estimated plastic shear strain plotted against the macroscopic plastic**  
 484 **strain, showing a significant plastic strain partitioning**

485 The macroscopic plastic strain, which was experimentally estimated using the crosshead  
 486 displacement, can be used to confirm the relevancy of the obtained estimates. A relationship with  
 487 the lattice rotation, which is extracted from the EBSD data, is searched in the following. To begin  
 488 with, the Schmid tensor relates the plastic shear rate  $\dot{\gamma}_i$  on slip system  $i$  with the plastic strain rate  
 489 tensor ( $\dot{\epsilon}_p$ ) as shown in equation (8):

490 
$$\dot{\epsilon}_p = \sum_{i=1}^N \frac{1}{2} (\mathbf{s}_i \otimes \mathbf{m}_i + \mathbf{m}_i \otimes \mathbf{s}_i) \dot{\gamma}_i \quad (8)$$

491 With  $\mathbf{s}_i$  the slip plane normal associated with slip system  $i$  in the sample frame and  $\mathbf{m}_i$  the slip  
 492 direction associated with slip system  $i$  in the sample frame. Assuming a negligible evolution of the  
 493 Schmid tensor, a direct relationship between the plastic strain in the loading direction ( $\epsilon_p$ ), the  
 494 apparent Schmid factor of the active slip system ( $SF$ ) and the plastic shear strain ( $\gamma$ ) is obtained after  
 495 time integration and shown in equation (9):

496 
$$\epsilon_p = SF \cdot \gamma \quad (9)$$

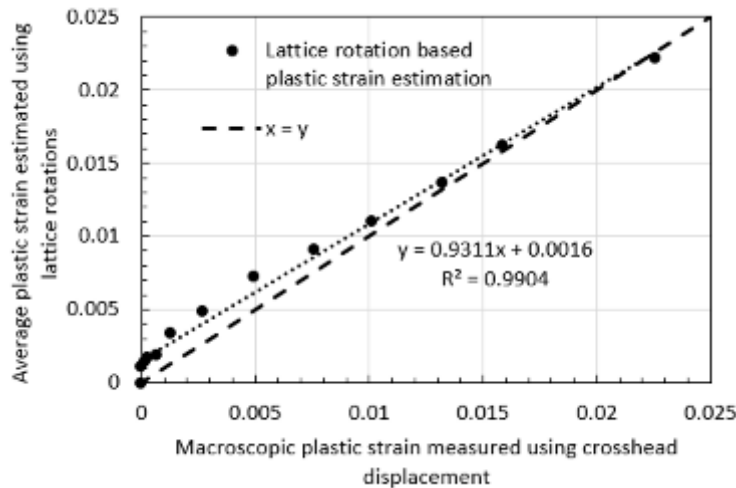
497 Then, a relationship between the macroscopic plastic strain ( $\bar{\epsilon}_p$ ) and the local plastic strain ( $\epsilon_p$ ) is  
 498 required. The macroscopic plastic strain ( $\bar{\epsilon}_p$ ) can be decomposed as follows:

499 
$$\bar{\epsilon}_p = \bar{\epsilon}_p^{Nodules} \cdot f_S^{Nodules} + \bar{\epsilon}_p^{Colonies} \cdot f_S^{Colonies} \quad (10)$$

500 With  $\bar{\epsilon}_p^{Nodules}$  the average plastic strain experienced by nodules,  $\bar{\epsilon}_p^{Colonies}$  the average plastic strain  
 501 experienced by colonies,  $f_S^{Nodules}$  the surface fraction associated with nodules and  $f_S^{Colonies}$  the  
 502 surface fraction associated with colonies. The average plastic strain in each type of microstructural  
 503 element (i.e. nodule or colony) is then calculated using measured lattice rotations. It is computed as  
 504 the arithmetic average of the plastic strain  $\epsilon_p$  over a given type of microstructural element, which is  
 505 expressed as follows using equations (7) and (9).

506 
$$\bar{\epsilon}_p^l = \frac{1}{\beta \cdot n_l} \cdot \sum_{k=1}^{n_l} SF_k \cdot \theta_k \quad (11)$$

507 With  $l$  being the type of microstructural element (i.e. nodule or colony),  $\beta$  the constant ( $\approx 28.6^\circ$ )  
 508 previously introduced which enables the conversion of shear strain into a magnitude of lattice  
 509 rotation,  $n_l$  the number of nodules or colonies considered,  $SF_k$  the Schmid factor of the nodule /  
 510 colony  $k$  and  $\theta_k$  the measured lattice rotation magnitude of nodule / colony  $k$ . Considering only the  
 511 microstructural elements associated with a basal or prismatic slip systems confidently identified, the  
 512 average plastic strain was estimated at each loading step using the angle of lattice rotations. The  
 513 resulting values are plotted in figure 8 with respect to the macroscopic plastic strain, which was  
 514 estimated using the crosshead displacement. The  $x = y$  line is also indicated.



515  
 516 **Figure 8: Average plastic strain, which is estimated using lattice rotations, plotted against the macroscopic**  
 517 **plastic strain, which is estimated using the crosshead displacement, showing a good agreement according to**  
 518 **the  $x = y$  line and the slope of the linear regression**

519 The average plastic strain estimated using lattice rotations is very close to the value obtained  
 520 using the crosshead displacement. In order to dismiss the influence of the angular offset in the elastic  
 521 regime, which is composed of rigid body and elastic rotations, a linear regression was applied. The  
 522 resulting slope is about 0.93, which is very close to 1. This very good agreement shows that a semi-  
 523 quantitative estimation of the plastic strain at the microstructural scale (i.e. for a set of grains) can be  
 524 performed using the presently proposed procedure. Further investigations are required for a  
 525 thorough assessment of the accuracy of this procedure for both individual and sets of grains.  
 526 Notably, the macroscopic strain estimation procedure could be improved using digital image  
 527 correlation or strain gages. In addition, non-deforming nodules, or colonies, have not been  
 528 considered. These points are left for future work.

529 **4.3 Lattice rotations and strain partitioning in Ti-6Al-4V**

530 While the nodule size and the maximum Schmid factor failed at accounting for the  
 531 dispersions in the magnitude of lattice rotation relative to the initial orientation, strikingly different  
 532 behaviors were evidenced by differentiating microstructural elements (i.e. nodules and colonies) and  
 533 active slip modes (i.e. basal and prismatic slip). These results, which have been previously discussed  
 534 in terms of lattice rotation, are interpreted hereafter in terms of strain partitioning. In average, basal  
 535 slip is associated with higher angles of rotation than prismatic slip for a given macroscopic plastic  
 536 strain level. This observation suggests that, in average, a higher plastic strain magnitude is  
 537 experienced by a microstructural element deforming by basal slip than by a similar microstructural

538 element deforming by prismatic slip. This is illustrated in figure 7 in terms of apparent plastic shear  
539 strain. Hence, plastic strain seems to be heterogeneously distributed depending on the active slip  
540 mode. This characteristic might be a consequence of the activation of basal slip at lower applied  
541 stress than prismatic slip [10,37,44]. However, the differences in CRSS values are small, i.e. typically a  
542 few percents [4,44,45]. A different strain hardening/softening behavior depending on the slip system  
543 considered might also significantly contribute to the strain partitioning. Prior studies based on  
544 experimental observations revealed a more pronounced strain softening for basal slip than for  
545 prismatic slip [46,47]. This characteristic might also significantly contribute to the differences in  
546 rotation and deformation behaviors at the grain scale.

547 Similarly, lattice rotation data suggests a marked strain partitioning between nodules and  
548 colonies. As illustrated in figure 7, the magnitude of average plastic strain in colonies appear lower  
549 than in nodules. The slow increase in plastic strain experienced by colonies is an evidence of the  
550 impediment of dislocation motion by  $\beta$  layers. Moreover, the basal / prismatic related strain  
551 partitioning, which is marked in nodules, appears significantly reduced in colonies. This observation  
552 results from interactions of dislocations of basal or prismatic slip systems with  $\beta$  layers. A more  
553 mechanistic understanding of these observations and of the effect on the heterogeneity of  
554 mechanical fields requires additional experimental characterizations as well as numerical  
555 simulations.

556 Over the last decades, much efforts have been put into CRSS estimation in order to obtain  
557 realistic crystal plasticity simulations [4,34,44]. As pointed out in a recent study [48], little data is  
558 available about the deformation behavior beyond slip initiation. In this context, lattice rotation data  
559 extracted using in situ EBSD are obviously valuable inputs for polycrystal plasticity simulations. Direct  
560 comparison of lattice rotation data with simulation results and parameter optimization is on-going  
561 for a quantitative assessment of strain partitioning. This constitutes a key milestone in a  
562 microstructure optimization framework as strain partitioning is well-known to have important  
563 consequences on the material performance through stress redistribution and slip induced damage  
564 processes [49-51].

565

## 566 5 Conclusions

567 Lattice rotations were characterized in situ during tensile deformation of a Ti-6Al-4V  
568 specimen using EBSD. A direct relation with plastic deformation at the microstructure scale was  
569 evidenced. To begin with, the rotation axis was used for the identification of the active slip system.  
570 The good agreement with a conventional slip trace analysis revealed a consistent identification of  
571 operating slip systems while complementary information, such as the slip direction, could be  
572 obtained. It enabled to demonstrate the widespread assumption that the basal slip traces most often  
573 corresponds to the slip system with the highest Schmid factor. This analysis also revealed a dominant  
574 contribution of intragranular plastic slip to the global lattice rotation behavior. In contrast, the  
575 contribution of rigid body rotations appears as secondary in the present conditions. Besides, the  
576 magnitude of the lattice rotation relative to the initial orientation exhibits a linear relationship with  
577 the plastic strain. This relation, which could be expected from classical crystal plasticity laws, offers  
578 insights into a direct quantification of the plastic strain at the microstructure scale using lattice  
579 rotation data. In agreement with previous investigations, a marked strain partitioning was evidenced  
580 between nodules and colonies. The operating slip mode was also identified as a factor of prime  
581 influence on strain partitioning. Nodules with operating basal slip experience, in average, a higher

582 plastic strain magnitude than nodules with operating prismatic slip. This heterogeneous strain  
583 distribution seems mitigated in colonies.

584

585 Declarations of interest: none

586

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684

685 **7 Appendix I**

686 The analysis of deformation processes described in the present work is based on averaging to  
687 reduce uncertainty in orientation measurement using conventional EBSD characterization. Considering  
688 conventional EBSD measurements and assuming a standard deviation of about 0.5° for individual  
689 measurements [], the standard deviation of the average orientation would be about 0.02° since the nodules  
690 presently considered contain at least 500 data points. This was experimentally confirmed by characterizing the  
691 same region twice using the same EBSD settings as given previously. The misorientation between the average  
692 orientations of a given grain was calculated using the two sets of orientation data. These values are reported in  
693 table A.1. The average misorientation is about 0.02° and the maximum is about 0.05°. This is consistent with  
694 the order of magnitude previously mentioned.

695

|           |        |
|-----------|--------|
| Nodule 1  | 0.002° |
| Nodule 2  | 0.007° |
| Nodule 3  | 0.021° |
| Nodule 4  | 0.042° |
| Nodule 5  | 0.011° |
| Nodule 6  | 0.033° |
| Nodule 7  | 0.041° |
| Nodule 8  | 0.012° |
| Nodule 9  | 0.014° |
| Nodule 10 | 0.021° |
| Nodule 11 | 0.013° |
| Nodule 12 | 0.024° |
| Nodule 13 | 0.023° |
| Nodule 14 | 0.009° |
| Nodule 15 | 0.004° |
| Nodule 16 | 0.024° |
| Nodule 17 | 0.024° |
| Nodule 18 | 0.034° |
| Nodule 19 | 0.029° |
| Nodule 20 | 0.027° |
| Nodule 21 | 0.010° |
| Nodule 22 | 0.024° |
| Nodule 23 | 0.020° |
| Nodule 24 | 0.023° |
| Nodule 25 | 0.022° |
| Nodule 26 | 0.029° |

|                |               |
|----------------|---------------|
| Nodule 27      | 0.010°        |
| Nodule 28      | 0.022°        |
| Nodule 29      | 0.020°        |
| Nodule 30      | 0.016°        |
| Nodule 31      | 0.031°        |
| Nodule 32      | 0.020°        |
| Nodule 33      | 0.022°        |
| Nodule 34      | 0.011°        |
| Nodule 35      | 0.023°        |
| Nodule 36      | 0.022°        |
| Nodule 37      | 0.031°        |
| Nodule 38      | 0.025°        |
| Nodule 39      | 0.033°        |
| Nodule 40      | 0.012°        |
| Nodule 41      | 0.024°        |
| Nodule 42      | 0.025°        |
| Nodule 43      | 0.011°        |
| Nodule 44      | 0.026°        |
| Nodule 45      | 0.029°        |
| Nodule 46      | 0.030°        |
| Nodule 47      | 0.033°        |
| Nodule 48      | 0.043°        |
| Nodule 49      | 0.016°        |
| Nodule 50      | 0.024°        |
| Nodule 51      | 0.035°        |
| Nodule 52      | 0.045°        |
| <b>Average</b> | <b>0.023°</b> |
| <b>Maximum</b> | <b>0.045°</b> |

696 **Table A.1 Misorientation between the average orientations of 52 nodules resulting of two EBSD characterizations of the**  
697 **same region. This is indicative of the precision of the orientation measurements.**  
698

699 The lack of certainty of the rotation axis was then investigated with a special focus on the effect on  
700 the determination of the slip induced rotation axis. Rotations of 0.1°, 0.2°, 0.4° and 1° about [0001] of the  
701 hexagonal close packed lattice were applied to the orientations of the second set of orientation. This is  
702 equivalent to the rotations induced by the operation of prismatic slip. Finally the rotation of slip induced  
703 rotation axes was calculated between the first set of orientations and the second set that includes an applied  
704 rotation. These values are reported in table A.2. Any rotation magnitude leads to a minimum rotation  
705 magnitude of the B1, B2 or B3 axes higher than the maximum rotation magnitude of the P rotation axis. This  
706 reveals a proper determination of the [0001] rotation axis (based on the lowest rotation magnitude). Hence,  
707 the use of averaged orientations enables to avoid lack of certainty of the rotation axis issues for prediction of  
708 operating slip systems associated with rotation magnitudes as low as 0.1°. Increasing the number of slip  
709 systems (i.e. the number of axes) or reducing the number of individual EBSD measurements per grain would  
710 impair the confidence in prediction and the precision level.  
711

| Rotation<br>Axis | 0°    |       |       |       | 0.1°  |       |       |       | 0.2°  |       |       |       | 0.4°  |       |       |       | 1°    |       |       |       |
|------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|                  | B1    | B2    | B3    | P     | B1    | B2    | B3    | P     | B1    | B2    | B3    | P     | B1    | B2    | B3    | P     | B1    | B2    | B3    | P     |
| Nodule 1         | 0.007 | 0.006 | 0.007 | 0.001 | 0.107 | 0.106 | 0.107 | 0.001 | 0.207 | 0.206 | 0.206 | 0.001 | 0.406 | 0.406 | 0.406 | 0.001 | 1.006 | 1.006 | 1.007 | 0.001 |
| Nodule 2         | 0.008 | 0.004 | 0.007 | 0.007 | 0.095 | 0.096 | 0.096 | 0.007 | 0.196 | 0.196 | 0.196 | 0.007 | 0.396 | 0.396 | 0.396 | 0.007 | 0.996 | 0.996 | 0.996 | 0.007 |
| Nodule 3         | 0.017 | 0.019 | 0.017 | 0.009 | 0.116 | 0.116 | 0.116 | 0.009 | 0.216 | 0.216 | 0.217 | 0.009 | 0.416 | 0.417 | 0.416 | 0.009 | 1.016 | 1.016 | 1.016 | 0.009 |
| Nodule 4         | 0.007 | 0.037 | 0.031 | 0.039 | 0.101 | 0.108 | 0.106 | 0.039 | 0.201 | 0.205 | 0.203 | 0.039 | 0.401 | 0.403 | 0.402 | 0.039 | 1.001 | 1.002 | 1.001 | 0.039 |
| Nodule 5         | 0.011 | 0.010 | 0.003 | 0.012 | 0.098 | 0.098 | 0.097 | 0.012 | 0.198 | 0.198 | 0.197 | 0.012 | 0.398 | 0.398 | 0.397 | 0.012 | 0.997 | 0.998 | 0.997 | 0.012 |
| Nodule 6         | 0.029 | 0.030 | 0.030 | 0.010 | 0.129 | 0.129 | 0.129 | 0.010 | 0.229 | 0.229 | 0.229 | 0.010 | 0.429 | 0.429 | 0.429 | 0.010 | 1.029 | 1.029 | 1.029 | 0.010 |
| Nodule 7         | 0.041 | 0.023 | 0.018 | 0.041 | 0.112 | 0.107 | 0.106 | 0.041 | 0.208 | 0.206 | 0.205 | 0.041 | 0.406 | 0.405 | 0.405 | 0.041 | 1.005 | 1.005 | 1.005 | 0.041 |
| Nodule 8         | 0.007 | 0.001 | 0.007 | 0.009 | 0.100 | 0.101 | 0.101 | 0.009 | 0.200 | 0.201 | 0.201 | 0.009 | 0.400 | 0.401 | 0.401 | 0.009 | 1.000 | 1.001 | 1.000 | 0.009 |
| Nodule 9         | 0.006 | 0.011 | 0.013 | 0.013 | 0.105 | 0.106 | 0.107 | 0.013 | 0.206 | 0.206 | 0.206 | 0.013 | 0.406 | 0.406 | 0.406 | 0.013 | 1.006 | 1.006 | 1.006 | 0.013 |
| Nodule 10        | 0.004 | 0.016 | 0.019 | 0.021 | 0.101 | 0.103 | 0.103 | 0.021 | 0.201 | 0.202 | 0.202 | 0.021 | 0.401 | 0.402 | 0.402 | 0.021 | 1.001 | 1.002 | 1.002 | 0.021 |
| Nodule 11        | 0.005 | 0.013 | 0.008 | 0.013 | 0.100 | 0.101 | 0.100 | 0.013 | 0.200 | 0.200 | 0.200 | 0.013 | 0.400 | 0.400 | 0.400 | 0.013 | 0.999 | 1.000 | 1.000 | 0.013 |
| Nodule 12        | 0.003 | 0.021 | 0.021 | 0.024 | 0.097 | 0.099 | 0.099 | 0.024 | 0.197 | 0.198 | 0.198 | 0.024 | 0.397 | 0.397 | 0.397 | 0.024 | 0.997 | 0.997 | 0.997 | 0.024 |
| Nodule 13        | 0.020 | 0.018 | 0.002 | 0.022 | 0.103 | 0.103 | 0.101 | 0.022 | 0.202 | 0.202 | 0.201 | 0.022 | 0.401 | 0.402 | 0.401 | 0.022 | 1.001 | 1.002 | 1.001 | 0.022 |

|           |       |       |       |       |                       |       |          |       |                       |       |          |       |                       |       |          |       |                       |       |          |       |
|-----------|-------|-------|-------|-------|-----------------------|-------|----------|-------|-----------------------|-------|----------|-------|-----------------------|-------|----------|-------|-----------------------|-------|----------|-------|
| Nodule 14 | 0.008 | 0.002 | 0.008 | 0.009 | 0.098                 | 0.098 | 0.098    | 0.009 | 0.198                 | 0.197 | 0.198    | 0.009 | 0.398                 | 0.397 | 0.398    | 0.009 | 0.998                 | 0.997 | 0.998    | 0.009 |
| Nodule 15 | 0.004 | 0.006 | 0.005 | 0.005 | 0.096                 | 0.096 | 0.096    | 0.005 | 0.196                 | 0.196 | 0.196    | 0.005 | 0.396                 | 0.396 | 0.396    | 0.005 | 0.996                 | 0.996 | 0.996    | 0.005 |
| Nodule 16 | 0.013 | 0.023 | 0.010 | 0.023 | 0.103                 | 0.105 | 0.103    | 0.023 | 0.203                 | 0.204 | 0.203    | 0.023 | 0.403                 | 0.403 | 0.403    | 0.023 | 1.003                 | 1.003 | 1.002    | 0.023 |
| Nodule 17 | 0.022 | 0.013 | 0.017 | 0.019 | 0.091                 | 0.089 | 0.090    | 0.019 | 0.190                 | 0.188 | 0.190    | 0.019 | 0.389                 | 0.388 | 0.389    | 0.019 | 0.989                 | 0.988 | 0.989    | 0.019 |
| Nodule 18 | 0.031 | 0.021 | 0.010 | 0.031 | 0.109                 | 0.106 | 0.105    | 0.031 | 0.207                 | 0.205 | 0.204    | 0.031 | 0.406                 | 0.405 | 0.404    | 0.031 | 1.005                 | 1.004 | 1.004    | 0.031 |
| Nodule 19 | 0.021 | 0.023 | 0.022 | 0.010 | 0.121                 | 0.122 | 0.121    | 0.010 | 0.221                 | 0.222 | 0.221    | 0.010 | 0.421                 | 0.421 | 0.421    | 0.010 | 1.021                 | 1.022 | 1.021    | 0.010 |
| Nodule 20 | 0.021 | 0.022 | 0.022 | 0.007 | 0.079                 | 0.079 | 0.080    | 0.007 | 0.179                 | 0.179 | 0.180    | 0.007 | 0.379                 | 0.379 | 0.379    | 0.007 | 0.979                 | 0.979 | 0.979    | 0.007 |
| Nodule 21 | 0.008 | 0.001 | 0.008 | 0.009 | 0.101                 | 0.101 | 0.101    | 0.009 | 0.201                 | 0.201 | 0.201    | 0.009 | 0.401                 | 0.401 | 0.401    | 0.009 | 1.000                 | 1.001 | 1.001    | 0.009 |
| Nodule 22 | 0.024 | 0.024 | 0.024 | 0.004 | 0.076                 | 0.077 | 0.076    | 0.004 | 0.176                 | 0.176 | 0.176    | 0.004 | 0.376                 | 0.376 | 0.376    | 0.004 | 0.976                 | 0.976 | 0.976    | 0.004 |
| Nodule 23 | 0.016 | 0.016 | 0.016 | 0.004 | 0.116                 | 0.116 | 0.116    | 0.004 | 0.216                 | 0.216 | 0.216    | 0.004 | 0.416                 | 0.416 | 0.416    | 0.004 | 1.016                 | 1.016 | 1.016    | 0.004 |
| Nodule 24 | 0.012 | 0.021 | 0.022 | 0.021 | 0.112                 | 0.113 | 0.114    | 0.021 | 0.212                 | 0.213 | 0.213    | 0.021 | 0.412                 | 0.413 | 0.412    | 0.021 | 1.012                 | 1.012 | 1.013    | 0.021 |
| Nodule 25 | 0.018 | 0.026 | 0.021 | 0.020 | 0.117                 | 0.119 | 0.117    | 0.020 | 0.217                 | 0.218 | 0.217    | 0.020 | 0.417                 | 0.417 | 0.417    | 0.020 | 1.017                 | 1.017 | 1.017    | 0.020 |
| Nodule 26 | 0.007 | 0.021 | 0.027 | 0.028 | 0.104                 | 0.106 | 0.107    | 0.028 | 0.204                 | 0.204 | 0.205    | 0.028 | 0.403                 | 0.404 | 0.404    | 0.028 | 1.004                 | 1.004 | 1.003    | 0.028 |
| Nodule 27 | 0.009 | 0.002 | 0.008 | 0.010 | 0.101                 | 0.101 | 0.101    | 0.010 | 0.201                 | 0.201 | 0.201    | 0.010 | 0.401                 | 0.401 | 0.401    | 0.010 | 1.001                 | 1.001 | 1.001    | 0.010 |
| Nodule 28 | 0.009 | 0.021 | 0.013 | 0.021 | 0.098                 | 0.100 | 0.099    | 0.021 | 0.197                 | 0.199 | 0.198    | 0.021 | 0.397                 | 0.398 | 0.398    | 0.021 | 0.998                 | 0.998 | 0.998    | 0.021 |
| Nodule 29 | 0.007 | 0.020 | 0.015 | 0.021 | 0.097                 | 0.098 | 0.098    | 0.021 | 0.197                 | 0.197 | 0.197    | 0.021 | 0.397                 | 0.397 | 0.397    | 0.021 | 0.997                 | 0.997 | 0.997    | 0.021 |
| Nodule 30 | 0.012 | 0.008 | 0.016 | 0.014 | 0.093                 | 0.093 | 0.093    | 0.014 | 0.193                 | 0.193 | 0.193    | 0.014 | 0.392                 | 0.393 | 0.392    | 0.014 | 0.993                 | 0.992 | 0.992    | 0.014 |
| Nodule 31 | 0.027 | 0.020 | 0.030 | 0.024 | 0.083                 | 0.080 | 0.084    | 0.024 | 0.181                 | 0.180 | 0.182    | 0.024 | 0.381                 | 0.380 | 0.381    | 0.024 | 0.980                 | 0.980 | 0.981    | 0.024 |
| Nodule 32 | 0.019 | 0.017 | 0.018 | 0.008 | 0.083                 | 0.083 | 0.083    | 0.008 | 0.183                 | 0.183 | 0.183    | 0.008 | 0.383                 | 0.383 | 0.383    | 0.008 | 0.983                 | 0.983 | 0.983    | 0.008 |
| Nodule 33 | 0.013 | 0.019 | 0.017 | 0.015 | 0.112                 | 0.113 | 0.113    | 0.015 | 0.212                 | 0.213 | 0.213    | 0.015 | 0.412                 | 0.412 | 0.412    | 0.015 | 1.012                 | 1.013 | 1.012    | 0.015 |
| Nodule 34 | 0.007 | 0.007 | 0.011 | 0.009 | 0.095                 | 0.095 | 0.095    | 0.009 | 0.195                 | 0.195 | 0.195    | 0.009 | 0.395                 | 0.395 | 0.394    | 0.009 | 0.995                 | 0.995 | 0.994    | 0.009 |
| Nodule 35 | 0.016 | 0.020 | 0.020 | 0.013 | 0.083                 | 0.084 | 0.084    | 0.013 | 0.184                 | 0.184 | 0.184    | 0.013 | 0.384                 | 0.384 | 0.384    | 0.013 | 0.984                 | 0.984 | 0.984    | 0.013 |
| Nodule 36 | 0.021 | 0.022 | 0.018 | 0.013 | 0.083                 | 0.083 | 0.082    | 0.013 | 0.182                 | 0.182 | 0.182    | 0.013 | 0.382                 | 0.382 | 0.382    | 0.013 | 0.982                 | 0.982 | 0.982    | 0.013 |
| Nodule 37 | 0.028 | 0.024 | 0.007 | 0.029 | 0.098                 | 0.097 | 0.094    | 0.029 | 0.196                 | 0.196 | 0.194    | 0.029 | 0.395                 | 0.395 | 0.394    | 0.029 | 0.995                 | 0.995 | 0.994    | 0.029 |
| Nodule 38 | 0.015 | 0.028 | 0.021 | 0.026 | 0.113                 | 0.116 | 0.114    | 0.026 | 0.213                 | 0.215 | 0.214    | 0.026 | 0.413                 | 0.414 | 0.413    | 0.026 | 1.013                 | 1.013 | 1.013    | 0.026 |
| Nodule 39 | 0.021 | 0.031 | 0.032 | 0.027 | 0.121                 | 0.124 | 0.123    | 0.027 | 0.221                 | 0.222 | 0.222    | 0.027 | 0.421                 | 0.422 | 0.422    | 0.027 | 1.021                 | 1.021 | 1.021    | 0.027 |
| Nodule 40 | 0.011 | 0.011 | 0.012 | 0.006 | 0.090                 | 0.089 | 0.090    | 0.006 | 0.190                 | 0.189 | 0.190    | 0.006 | 0.389                 | 0.389 | 0.390    | 0.006 | 0.989                 | 0.989 | 0.989    | 0.006 |
| Nodule 41 | 0.001 | 0.021 | 0.020 | 0.024 | 0.100                 | 0.102 | 0.101    | 0.024 | 0.199                 | 0.201 | 0.200    | 0.024 | 0.400                 | 0.400 | 0.400    | 0.024 | 1.000                 | 1.000 | 1.000    | 0.024 |
| Nodule 42 | 0.023 | 0.011 | 0.023 | 0.024 | 0.091                 | 0.089 | 0.091    | 0.024 | 0.190                 | 0.188 | 0.190    | 0.024 | 0.390                 | 0.389 | 0.390    | 0.024 | 0.989                 | 0.989 | 0.990    | 0.024 |
| Nodule 43 | 0.015 | 0.011 | 0.009 | 0.013 | 0.093                 | 0.092 | 0.093    | 0.013 | 0.192                 | 0.193 | 0.192    | 0.013 | 0.393                 | 0.392 | 0.392    | 0.013 | 0.993                 | 0.993 | 0.992    | 0.013 |
| Nodule 44 | 0.018 | 0.019 | 0.023 | 0.016 | 0.084                 | 0.084 | 0.085    | 0.016 | 0.183                 | 0.183 | 0.184    | 0.016 | 0.383                 | 0.383 | 0.383    | 0.016 | 0.983                 | 0.984 | 0.983    | 0.016 |
| Nodule 45 | 0.024 | 0.029 | 0.020 | 0.022 | 0.082                 | 0.084 | 0.081    | 0.022 | 0.182                 | 0.182 | 0.181    | 0.022 | 0.381                 | 0.381 | 0.381    | 0.022 | 0.981                 | 0.981 | 0.981    | 0.022 |
| Nodule 46 | 0.028 | 0.029 | 0.029 | 0.009 | 0.073                 | 0.073 | 0.073    | 0.009 | 0.173                 | 0.173 | 0.172    | 0.009 | 0.373                 | 0.373 | 0.373    | 0.009 | 0.973                 | 0.972 | 0.972    | 0.009 |
| Nodule 47 | 0.019 | 0.031 | 0.025 | 0.026 | 0.117                 | 0.119 | 0.118    | 0.026 | 0.217                 | 0.218 | 0.218    | 0.026 | 0.417                 | 0.417 | 0.417    | 0.026 | 1.017                 | 1.017 | 1.016    | 0.026 |
| Nodule 48 | 0.042 | 0.041 | 0.027 | 0.036 | 0.131                 | 0.131 | 0.127    | 0.036 | 0.229                 | 0.229 | 0.227    | 0.036 | 0.428                 | 0.428 | 0.427    | 0.036 | 1.028                 | 1.028 | 1.027    | 0.036 |
| Nodule 49 | 0.017 | 0.009 | 0.013 | 0.015 | 0.093                 | 0.092 | 0.092    | 0.015 | 0.193                 | 0.192 | 0.192    | 0.015 | 0.392                 | 0.392 | 0.392    | 0.015 | 0.992                 | 0.992 | 0.992    | 0.015 |
| Nodule 50 | 0.002 | 0.021 | 0.019 | 0.023 | 0.100                 | 0.102 | 0.103    | 0.023 | 0.201                 | 0.202 | 0.201    | 0.023 | 0.400                 | 0.401 | 0.401    | 0.023 | 1.001                 | 1.001 | 1.001    | 0.023 |
| Nodule 51 | 0.036 | 0.028 | 0.021 | 0.031 | 0.087                 | 0.084 | 0.082    | 0.031 | 0.184                 | 0.182 | 0.182    | 0.031 | 0.383                 | 0.382 | 0.382    | 0.031 | 0.982                 | 0.982 | 0.981    | 0.031 |
| Nodule 52 | 0.034 | 0.023 | 0.040 | 0.035 | 0.083                 | 0.079 | 0.085    | 0.035 | 0.180                 | 0.179 | 0.181    | 0.035 | 0.379                 | 0.378 | 0.380    | 0.035 | 0.979                 | 0.978 | 0.979    | 0.035 |
|           |       |       |       |       | Min<br>B1<br>B2<br>B3 | 0.073 | Max<br>P | 0.041 | Min<br>B1<br>B2<br>B3 | 0.172 | Max<br>P | 0.041 | Min<br>B1<br>B2<br>B3 | 0.373 | Max<br>P | 0.041 | Min<br>B1<br>B2<br>B3 | 0.972 | Max<br>P | 0.041 |

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**Table A.2 The rotation of slip induced rotation axes (in degrees) between the first set of orientations and the second set of orientation that includes an applied rotation for 52 nodules. For any rotation magnitude, no overlap was noticed between the minimum among B1, B2 and B3 axes rotation magnitudes and the P axis rotation magnitude, which indicates an accurate prediction of the operating deformation systems.**