

1 Local slip activities in polycrystalline α -Ti depending on textures and strain rates

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1 **Abstract**

2 It is possible that strain localization in polycrystalline α -Ti leads to the fracture, and it is
3 crucial to evaluate the local slip activities for individual slip systems depending on their
4 textures and loading conditions. In this study, the effects of textures and strain rates on
5 local slip activities were investigated using the crystal plasticity finite element method.
6 For the analysis, microstructural models of α -Ti with the following three textures were
7 employed: aggregates of (0001) axes are (i) splitting in rolling direction (RD-split texture),
8 (ii) splitting in transverse direction (TD-split texture), and (iii) aligned in normal direction
9 (basal texture). For each texture model, two variations in the crystal orientation
10 distributions were considered, namely, small and large scatterings of crystal orientations
11 in the (0001) axes by normal random numbers. The differences in the strain rate
12 sensitivities of the critical resolved shear stresses (CRSSs) among slip systems were also
13 considered. Tensile loading was applied by a forced displacement in the RD with two
14 strain rate conditions of $1.0 \times 10^{-4} \text{ s}^{-1}$ and $1.0 \times 10^{-1} \text{ s}^{-1}$. Local non-prismatic slips were
15 easier to operate in the models with basal and RD-split textures than with the TD-split
16 texture. The slip strains for non-prismatic slip systems were higher at higher strain rates,
17 while activities in the prismatic slips decreased with an increase in strain rates. The
18 mechanism of the exchange of slip system activities can be explained by strain

1 redistribution between hard and soft regions and changes in CRSS as a function of strain
2 rates.

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4 **KEYWORDS:** crystal plasticity analysis; titanium; α -phase; strain rate; crystallographic
5 textures; heterogeneous deformation; slip activity

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1 **1. Introduction**

2 Titanium and its alloys with excellent mechanical properties have been used as
3 structural materials in various fields, such as aerospace, medicine, and sports equipment
4 [1,2]. Thus, understanding fracture mechanisms are crucial for enhancement of the safety
5 and performance of the products. The fracture is related to the microscopic deformation
6 mechanisms. In α titanium (α -Ti), soft grains (which easily undergo plastic deformation)
7 and hard grains (which do not easily undergo plastic deformation) exist. Stress and strain
8 are redistributed between the soft and hard grains during the deformation, and it is
9 possible that the stress and strain concentration induced by the inhomogeneous
10 deformation lead to the fracture [3–5].

11 The ease of plastic deformation in each grain is strongly affected by critical
12 resolved shear stress (CRSS) as well as crystallographic orientations. Slip systems in α -
13 Ti with hcp structure are basal slip systems (Bsl $\langle a \rangle$), prismatic $\langle a \rangle$ slip systems (Pri $\langle a \rangle$
14 $\langle a \rangle$), 1st order pyramidal $\langle a \rangle$ slip systems (Pyr $\langle a \rangle$), 1st order pyramidal $\langle c + a \rangle$ (Pyr-
15 $\langle c + a \rangle$), and 2nd order pyramidal $\langle c+a \rangle$. The CRSSs are different among slip systems,
16 and the difference strongly affect the deformation mechanism. In recent years, crystal
17 plasticity analysis, which accurately represent deformation in crystal grain level as well
18 as macroscopic stress-strain relationships, is typically employed to investigate the

1 deformation mechanisms [6–14]. The relationship between inhomogeneous deformation
2 and CRSS ratio has been investigated by crystal plasticity analysis. Baudoin et al. (2019)
3 represented deformation of commercially pure titanium (CP-Ti) by the crystal plasticity
4 analysis, and reported that the heterogeneous strain distribution is attributed to the CRSS
5 ratio [14]. Kawano et al. investigated strain distributions in polycrystalline α -Ti using
6 crystal plasticity analysis and revealed that strain concentration can appear because of
7 strain redistribution between soft and hard regions [13,15]; an imbalance in the CRSS
8 ratio among slip systems induces strain concentration [13].

9 The CRSS ratio in α -Ti changes with strain rates as well as the chemical
10 composition and processing history. In α -Ti, the strain rate sensitivity of CRSS for Pri < a >
11 a > is greater than that of the Bsl < a > [16,17]. Okamoto et al. conducted a crystal
12 plasticity analysis to study the uniaxial deformation of polycrystalline α -Ti with an RD-
13 split texture, considering the differences in strain rate sensitivities among slip systems
14 [18]. With increases in strain rates, Pri < a > activity can decrease in the most of volumes
15 in the specimen while non-Pri < a >, such as Bsl < a > and Pyr < a > increase locally.
16 However, the above study focused on the strain redistribution mechanism occurring in
17 the RD-split texture, and the activities of individual slip systems in other textures remain
18 unknown. However, the activities of slip systems depending on microstructures can be

1 quantitatively evaluated by crystal plasticity analysis [6,8,13,14,19,20]. Further, this
2 method can also be used to evaluate the dependence of slip system activities depending
3 on the textures and strain rates in polycrystalline α -Ti [13]. Notably, crystal plasticity
4 analysis with a rate-dependent single crystal constitutive equation reasonably predicts
5 strain-rate dependent polycrystalline behavior based on the experimentally reported strain
6 rate sensitivity of single crystal alpha-Ti [16,17]. Regardless of the capability of the
7 prediction, systematic study of strain rate sensitivity of textured poly-crystalline alpha-Ti
8 has not been performed so far. This study focuses on the investigation of activity of slip systems
9 in polycrystalline level.

10 Crystallographic textures typically observed in α -Ti are shown in Table 1, and
11 change with chemical composition and processing history [21]. As stated above,
12 systematic investigation of slip system activities in individual textures has not been
13 investigated in α -Ti. In this study, we investigated the activities of individual slip systems
14 in polycrystalline α -Ti depending on strain rates and textures using crystal plasticity
15 analysis. This paper is organized as follows. First, we explain the geometric model and
16 crystal orientations for crystal plasticity analysis. We prepared three types of textures for
17 the analysis: (i) RD-split texture, (ii) TD-split texture in which aggregates of (0001) axis
18 divide in the TD, and (iii) basal texture in which the (0001) axes align in the direction

1 normal to the RD and TD (ND). Further, small and large scatterings of crystal orientations
2 were specified in each texture model. Second, we explain the method for the crystal
3 plasticity analysis employed in this study and the conditions for the analysis. Third, the
4 activities for individual slip systems depending on textures and strain rates are
5 demonstrated, and finally, we infer the conditions for crack initiation from the results of
6 local slip activation, which occur easily.

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9 **2. Geometric models for crystal plasticity analysis**

10 **2.1 Microstructure reproduction**

11 The geometric model representing the microstructure of polycrystalline α -Ti
12 employed in this study is shown in Fig. 1. Voronoi tessellation, which was used to
13 reproduce microstructures in polycrystalline materials [22][23][24][25], was employed to
14 build the model. A brief description of Voronoi tessellation employed in this study is as
15 follows: First, the material for the analysis is assumed. The points for crystal nucleation,
16 where the number corresponds to crystal nuclei, are distributed within the material.
17 Second, all the volumes divided in the material are assumed to belong to individual
18 nearest nuclei, and then the regions consisting of divided volumes are classified by the

1 nuclei, where each classed region is assumed to be a crystal grain. The microstructures
2 built by this method correspond to those obtained under the condition that crystal nuclei
3 are generated simultaneously and grow isotropically. In this study, the size of the material
4 is $800.0\ \mu\text{m} \times 600.0\ \mu\text{m} \times 8.0\ \mu\text{m}$ and is divided into $100 \times 75 \times 1$ voxels. Five hundred
5 nuclei are randomly generated and grown isotropically within the material, and the
6 microstructure obtained under this condition is shown in Fig. 1. Increasing the number of
7 elements yields strain distributions with high resolution. However, if loss of information
8 on crystallographic orientation distributions is little, the strain distributions are not
9 strongly affected by the number of elements in crystal plasticity analysis [26].
10 Furthermore, in this study, we focus the current study on deformation behavior at the
11 polycrystalline level and consider the computational cost, which resulted in the above
12 number of elements adopted in the current analysis.

13

14 **2.2 Textures**

15 Crystal orientations are specified in individual grains of the geometric model
16 shown in Fig. 1. Six texture models were built as shown in Fig. 2. Typical textures
17 observed in α and near α -Ti are listed in Table 1 [21]. In this study, the axis orientations
18 for RD-split, TD-split, and basal textures were selected from Table 1. (0001) axes of basal,

1 T, and R textures are aligned in a particular direction, and their crystal orientation
2 distributions are the same with each other when their coordinate systems are rotated. Thus,
3 the basal texture is selected to represent basal, T, and R textures. Small and large
4 scatterings of crystal orientations are provided for the above three types of textures.
5 Crystal orientations are expressed by a set of Euler angles $(\varphi_1, \Phi, \varphi_2)$ defined by Bunge,
6 where φ_1 determines the rotation angle around (0001) axes and the direction of inclination
7 of (0001) axes, Φ determines the inclination angle of (0001) axes, and φ_2 determines the
8 rotation angle around (0001) axes. φ_1 , Φ , and φ_2 are assigned according to the orientations
9 described in Table 1. φ_2 is assigned by random numbers from 0° to 360° , and we employed
10 the following values: $(\varphi_1, \Phi, \varphi_2) = (90^\circ, \pm 20^\circ, 0 \text{ to } 360^\circ)$ in RD-split texture, $(0^\circ, \pm 30^\circ,$
11 $0^\circ \text{ to } 360^\circ)$ in TD-split texture, and $(\varphi_1, \Phi, \varphi_2) = (0^\circ, 0^\circ, 0^\circ \text{ to } 360^\circ)$ in basal texture, and
12 the scattering of the (0001) axes in each texture is given by normal random numbers. The
13 standard deviations for the random numbers were 10° and 40° . Models with small
14 scatterings are defined as SD10, while those with large scatterings are defined as SD40.
15 The pole figures for the textures obtained by the above conditions are shown in Fig. 2,
16 and Fig. 3 shows the distributions of Schmid factors for $\langle a \rangle$ slip systems for the tensile
17 direction, which are considered major active slip systems.

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2 **3. Methods for crystal plasticity analysis**

3 In this study, a CPFE method incorporating the framework developed by Peirce et
4 al. [27][28] was employed for deformation analysis. A brief description of the method is
5 as follows. The activation of slip systems is assumed to follow the Schmid law, and the
6 strain rate for each slip system is given by

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

9

10 where i , j , $\dot{\gamma}_0$, and τ correspond to the number of slip systems, shear slip rate, reference
11 shear strain rate, and resolved shear stress (RSS), respectively. m is the slip rate sensitivity
12 parameter; the CRSS changes more easily with the strain rate when m is large. In this
13 study, the differences in the strain rate sensitivities of CRSS for individual slip systems
14 are represented by different m values among slip systems. The value of g for Eq. (1) is
15 obtained from Voce-type hardening law [29][30]:

16

$$17 \quad \dot{g}^{(i)} = \frac{d\hat{\tau}}{d\Gamma} \sum_j h_{ij} \dot{\gamma}^{(j)}, \quad (2)$$

18

$$\hat{\tau}^{(i)} = \tau_0^{(i)} + (\tau_1^{(i)} + \theta_1^{(i)}\Gamma) \left\{ 1 - \exp\left(-\frac{\theta_0^{(i)}\Gamma}{\tau_1^{(i)}}\right) \right\}, \quad (3)$$

2

3 where Γ is the cumulative slip strain considering all slip systems and h_{ij} is the hardening
 4 matrix. τ_0 , τ_1 , θ_0 , and θ_1 are the parameters to represent the relationships between shear
 5 stress and shear strain.

6 **4. Conditions for crystal plasticity analysis**

7 The elastic constants of pure titanium [31], shown in Table 2, were employed for
 8 CPFEE analysis. The work hardening parameters are shown in Table 3, and the relationship
 9 between $\hat{\tau}$ and Γ is shown in Fig. 4a, where $\hat{\tau}$ determines the CRSS for each slip system.
 10 CRSSs in α -Ti vary not only with the chemical composition ²⁸⁾ but also with the
 11 processing history and conditions. Thus, the CRSS ratio may differ between α -Ti alloys
 12 even when their chemical compositions are the same [33]. In this study, CRSS values
 13 were determined as described by Warwick et al. [34] and Kawano et al. [13]. Twinning is
 14 assumed to be inactive as titanium alloys contain a substantial amount of O or >7.0% Al
 15 [2][35][36]. While it is possible that work softening occurs in <a> slip systems depending
 16 on the conditions in α -Ti [37][38], this study ignores the softening. Further, we assume
 17 that the work hardening is negligible in <a> slip systems and occurs slightly in <c + a
 18 > slip systems, as shown in Fig. 4a.

1 The values of m , which determine the strain rate sensitivities of CRSS, are listed in
2 Table 4. The m values for Bsl $\langle a \rangle$ and Pri $\langle a \rangle$ are determined based on the experimental
3 results obtained by Jun et al. [16] and Chatterjee et al. [17], and m for Pri $\langle a \rangle$ is larger
4 than that for Bsl $\langle a \rangle$. The m value of 0.02 was used for other slip systems employed in
5 CPFE analysis [14][33]. Thus, the m values for Pyr $\langle a \rangle$ and $\langle c + a \rangle$ slip systems were
6 not obtained experimentally. However, the activity for $\langle c + a \rangle$ slip systems is low owing
7 to the high CRSS, and the change in CRSS with strain rate is limited in the activity of \langle
8 $c + a \rangle$ slip systems. In contrast, previous reports [39][40] indicate that CRSS for Pyr $\langle a$
9 \rangle may be relatively low, and it is possible that its activation influences the activity of
10 other slip systems [13]. As stated above, the precise CRSS of Pyr $\langle a \rangle$ depending on the
11 strain rate is unknown. Thus, two conditions for Pyr $\langle a \rangle$ are employed in this study; the
12 first condition is that only Bsl $\langle a \rangle$ and Pri $\langle a \rangle$ are activated (BP condition), and the
13 second is that all slip systems are activated (AS condition). Under AS condition, while \langle
14 $c + a \rangle$ slip systems are activated, the activity is quite low because of high CRSS, and the
15 activation of $\langle c + a \rangle$ slip systems has a negligible impact on the activity of other slip
16 systems.

17 Fig. 4b shows the initial CRSSs for Bsl $\langle a \rangle$ and Pri $\langle a \rangle$ in a single α -Ti as a
18 function of the strain rates obtained by CPFE analysis [18]. The CRSSs for both slip

1 systems increase with increasing strain rates; however, the sensitivity of strain rates is
2 different between them, and the CRSSs are similar when the strain rate is high.

3 The boundary conditions employed for the CPFE analysis are shown in Fig. 1,
4 where the left-hand side plane perpendicular to the X-direction was fixed in the X-
5 direction, and a forced displacement in the X-direction was applied to the right-hand side
6 plane perpendicular to the X-direction. Two strain rate conditions were employed: (i) 1.0
7 $\times 10^{-4} \text{ s}^{-1}$ (low strain rate condition) and (ii) $1.0 \times 10^{-1} \text{ s}^{-1}$ (high strain rate condition). The
8 zero-stress condition is applied to other planes, except for those perpendicular to the X-
9 direction.

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12 **5. Results and discussions**

13 **5.1 Macroscopic stress–strain relationship**

14 Before investigating the microscopic strain concentration mechanisms, we
15 investigated the macroscopic stress–strain relationship depending on the textures and
16 strain rates. Fig. 5 shows the relationship between the nominal strain and stress. The yield
17 points increased with strain rates under all conditions. This reflects the increases of initial
18 CRSS with increasing strain rates as shown in Fig. 4b. This increase in yield points with

1 strain rates was also observed experimentally [41] while the strain rate dependency
2 obtained in the current analyses was stronger than that in the experiment. These stress–
3 strain relationships depending on strain rates were similar among the textures analyzed
4 for the current simulation conditions.

5 The effects of scattering of crystal orientation on the macroscopic stress–strain
6 relationship are small; however, the difference in flow stress between SD10 and SD40 is
7 larger in the RD-split texture than those in the TD-split and basal textures. This slight
8 difference among textures is derived from the activity of slip systems due to the difference
9 in Schmid factors between textures as shown in Fig. 3. Typically, the activation of $\text{Pri} <$
10 $\text{a} >$ would have larger effects on the macroscopic stress-strain relationships. We
11 quantitatively demonstrate the activity of each slip system in the next section.

12

13 **5.2 Activity of slip systems depending on textures and strain rates**

14 In this section, we investigate the activity of slip systems depending on the
15 textures and strain rates. The activity of the slip systems is investigated using the
16 distributions of slip strains in two-dimensional planes, followed by a more quantitative
17 investigation using the line profiles of slip strains. High strain was observed both within
18 and inner the grains. This will be related to the crystallographic orientation relationship

1 between grains [4][5]. However, in this study, we focus on the strain distribution at the
2 polycrystalline level and will systematically investigate the intragranular inhomogeneity
3 in the future works.

4 Fig. 6 shows the distributions of slip strain for the $\langle a \rangle$ slip systems under the
5 SD10 condition. The activities of the $\langle c + a \rangle$ slip systems are relatively low, and the
6 distributions are not shown. In the RD-split texture with the AS condition (Fig. 6a RD-
7 split texture), $\text{Pri} \langle a \rangle$ activity decreases with strain rates while the $\text{Pyr} \langle a \rangle$ activity
8 increases with the strain rates. Conversely, in RD-split texture with BP condition (Fig. 6b
9 RD-split texture), the activity of $\text{Bsl} \langle a \rangle$ increases with strain rates while the activity of
10 $\text{Pri} \langle a \rangle$ decreases with strain rates. This difference in activities is because the strain rate
11 sensitivity of CRSS for $\text{Pri} \langle a \rangle$ is higher than those for other slip systems, and the
12 deformation volume by activation of $\text{Pri} \langle a \rangle$ decreases with high strain rates. Thus, when
13 activity of $\text{Pri} \langle a \rangle$ decreases with strain rates, other slip systems are required to be
14 activated to supply the shortage of deformation volume arising from the decreasing
15 activity of $\text{Pri} \langle a \rangle$. The strain rate sensitivity of CRSS for $\text{Pyr} \langle a \rangle$ employed in this
16 study has an unclear physical basis, and its accuracy is unknown. However, deformation
17 analysis was performed under active and inactive conditions of $\text{Pyr} \langle a \rangle$, and the results
18 indicate the following. The activity of $\text{Pri} \langle a \rangle$ decreases with strain rates, while the

1 activity of non-Pri $\langle a \rangle$ increases with strain rates in the RD-split texture. In non-Pri $\langle a \rangle$
2 \rangle activation, Bsl $\langle a \rangle$ activity can be suppressed by Pyr $\langle a \rangle$ activation. A similar
3 tendency was observed by Okamoto et al. [18].

4 In contrast, under the conditions of TD-split and basal textures (Fig. 6), the activity
5 of Pri $\langle a \rangle$ is dominant. This variation is observed because the high Schmid factors for
6 Pri $\langle a \rangle$ in TD and basal textures with SD10 conditions (Fig. 3a) strongly affect the
7 activation of Pri $\langle a \rangle$ than large CRSS due to the strain rates. Therefore, while the
8 difference in strain rate sensitivities of CRSSs among slip systems may induce changes
9 in the activity of slip systems with strain rates, the tendency of the phenomena is different
10 depending on the textures.

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13 **5.3 Effects of variety of crystal orientations**

14 The scattering of crystal orientations occurs in actual textures, and the effects of
15 scattering on the activities of slip systems are investigated in this section. Fig. 7 shows
16 the distributions of slip strains when large scattering occurs in crystal orientations (i.e.,
17 the results obtained under SD40 condition). Activities of non-Pri $\langle a \rangle$ are higher under
18 SD40 condition (Fig. 7) than those under SD10 (Fig. 6). The activities of the slip systems

1 in the individual textures are presented below.

2 In RD-split texture, while the strain rate sensitivities of slip system activities were
3 similar between SD10 (Fig. 6) and SD40 (Fig. 7), slight variations in the distributions of
4 slip strains were observed. Specifically, the activities of Bsl $\langle a \rangle$ and Pyr $\langle a \rangle$ are greater
5 in SD40 than those in SD10. Typically, Bsl $\langle a \rangle$ was activated (Fig. 7) in TD-split and
6 basal textures with SD40, which was not observed in SD10 (Fig. 6), and the activities of
7 the system were higher at higher strain rates. This is because when large scattering occurs
8 in crystal orientations, non-Pri $\langle a \rangle$ are activated in TD-split, basal, and RD-split textures
9 and the activities of non-Pri $\langle a \rangle$ are higher with higher strain rates due to the strain rate
10 sensitivities of CRSSs.

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13 **5.4 Local slip and its relaxation by activation of Pyr $\langle a \rangle$ slip systems**

14 A quantitative evaluation of the activities in slip systems is conducted using line
15 profiles. Fig. 8 shows the line profiles of slip strain, where only the results with high
16 activity of non-Pri $\langle a \rangle$ are shown: the results of RD-split texture with SD10 and SD40,
17 and those of basal texture with SD40. The local activation of slip systems was observed
18 under the conditions shown in Fig. 8. Typically, strain concentration occurs more easily

1 in basal texture, which is caused by the scattering of aggregates of the (0001) axes. The
2 inclination of the (0001) axis in the basal texture increases the Schmid factor for Bsl $\langle a \rangle$
3 \rangle , and grains with a high Schmid factor are distributed within the specimen when the
4 scattering of (0001) axes are applied for grains. Strain tends to concentrate around such
5 scattered regions with high Schmid factor, which easily undergo plastic deformation due
6 to the strain redistribution mechanism between soft and hard regions [8][18]. In contrast,
7 volume with high Schmid factor for Bsl $\langle a \rangle$ in RD-split texture is larger than that for
8 basal texture as shown in Fig. 3, and the strain concentration of Bsl $\langle a \rangle$ is moderate in
9 RD-split texture, compared to basal texture (Fig. 8). Furthermore, this ease of strain
10 concentration has a strain rate dependency. Under all conditions in Fig. 8, slip strains of
11 Pri $\langle a \rangle$ decreased and that of Bsl $\langle a \rangle$ or Pyr $\langle a \rangle$ increased with an increase in strain
12 rates. That is, strain rates enhanced strain redistribution, and activities of non-Pri $\langle a \rangle$
13 increases locally by reducing activities in Pri $\langle a \rangle$ with an increase of strain rates.
14 However, it is noted that strain rate sensitivity of CRSS for Pyr $\langle a \rangle$ is unclear, and Pri
15 $\langle a \rangle$ may activate with high strain rate when the strain rate sensitivity of CRSS for Pyr
16 $\langle a \rangle$ is higher than that of Pri $\langle a \rangle$.

17 Next, the strain redistribution of non-Pri $\langle a \rangle$ with the strain rates is discussed.
18 Under AS condition (Fig. 8a), the activity of Pyr $\langle a \rangle$ increases with strain rates, while

1 that of Pri < a > decreases. Then, the change in that of Bsl <a> with strain rates is relatively
2 slight. In contrast, under PB condition (Fig. 8b), while Pri < a > activity decreases, the
3 peaks of slip strain for Bsl < a > increases with strain rates, indicated by arrows in Fig.
4 8b. That is, activation of Bsl < a > is suppressed by that of Pyr < a >, and the same
5 tendency was observed in Okamoto et al. [18].

6 Finally, we discuss the relationship between the above results and the crack
7 nucleation mechanism. Crack nucleation along slip planes for Bsl < a >, Pri < a >, and
8 Pyr < a > were commonly observed [41]. In bimodal Ti-64, cracks were observed in the
9 planes along the slip planes for Bsl < a > and Pri < a > [42]. Thus, cracks are nucleated
10 along the planes in which the activities of the slip systems are high. While twinning plays
11 an important role in crack nucleation in pure titanium and commercially pure titanium
12 under cyclic loading [43], the addition of a large amount of O or Al (above 7%) suppresses
13 twinning [2][35] [36]. O and Al increase the c/a ratio [36] [39][44][45], and differences
14 in the CRSS between Pri < a > and non-Pri < a > decreases by the addition of such alloying
15 elements. In this study, the CRSS for Pri < a > is close to that of Bsl < a >. Therefore, the
16 results of this study would represent deformation mechanism in α -Ti with a high c/a ratio.
17 In such α -Ti with an RD-split or basal texture, non-Pri < a > may activate locally under
18 RD tensile deformation, and the activity increases with strain rates. Under these

1 conditions, it is predicted that crack nucleation is induced by non-Pri $\langle a \rangle$ activation and
2 scattering of crystal orientations in textures.

3 **Importantly, the numerical results in this study should be experimentally confirmed**
4 **in the further study. In the experiment, texture, chemical composition and oxide**
5 **concentration, which could affect activities and strain rate sensitivity of each deformation**
6 **modes, must be carefully selected.**

7

8

9 **6. Conclusions**

10 In this study, we conducted CPFE analysis of uniaxial tensile deformation in
11 polycrystalline α -Ti with RD-split, TD-split, and basal textures. Small and large
12 scatterings of crystal orientations are provided in individual textures; models with small
13 and large scatterings are called SD10 and SD40, respectively. Differences in the strain
14 rate sensitivities for CRSSs for individual slip systems were incorporated in all analyses.
15 We investigated the relationship between the local activation of slip systems and effects
16 of textures and CRSS depending on strain rates. The results can be summarized as
17 follows:

18 1. The increase in macroscopic flow stress with strain rates was reproduced by CPFE

1 analysis. Scattering in crystal orientations has a negligible impact on the macroscopic
2 stress–strain relationship for all textures.

3 2. Scattering of the (0001) axes affected the local activation of the slip systems. Typically,
4 basal slip systems activity is locally high in basal texture when large scattering occurs.

5 3. The activity of Pri $\langle a \rangle$ decreased with increasing strain rates. In contrast, non-Pri $\langle a \rangle$
6 $\langle a \rangle$ is activated with increasing strain rates. While strain rate sensitivity of CRSS for
7 Pyr $\langle a \rangle$ slip systems is unknown, the activity of Bsl $\langle a \rangle$ increases with strain rates
8 on the condition that Pyr $\langle a \rangle$ activity is high, and decreases with strain rates on the
9 condition that Pyr $\langle a \rangle$ activity is low. Thus, Activation of Pyr $\langle a \rangle$ suppresses that
10 of Bsl $\langle a \rangle$. However, the exchange of activities between slip systems does not occur
11 depending on the textures and CRSS ratios owing to the low CRSSs and high Schmid
12 factors for Pri $\langle a \rangle$.

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3 **Data availability**

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

6

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17 **Figure and table captions**

18 Fig. 1 Polycrystalline model of α -Ti.

- 1 Fig. 2 Pole figures of (a) SD10 model and (b) SD40 model with RD-split, TD-split, and
2 basal textures.
- 3 Fig. 3 Distributions of Schmid factors in (a) SD10 and (b) SD40 models.
- 4 Fig. 4 (a) $\hat{\tau}$ for each slip system as a function of cumulative slip strain and (b) initial
5 CRSSs for Bsl $\langle a \rangle$ and Pri $\langle a \rangle$ depending on the strain rates [18].
- 6 Fig. 5 Profiles showing the relationship between nominal stress and strain obtained by
7 models with RD-split texture (a, d), TD-split texture (b, e), and basal texture (c,
8 f). Activation of Pyr $\langle a \rangle$ is considered in (a–c) and not considered in (d–f).
- 9 Fig. 6 Slip strain distributions when SD10 models are employed, and nominal strain is
10 2.0 %; (a) AS condition and (b) BP condition.
- 11 Fig. 7 Slip strain distributions when SD40 models are employed and nominal strain is
12 2.0 %; (a) AS condition and (b) BP condition.
- 13 Fig. 8 Line profiles of slip strain along X_1 – X_2 in Fig. 1 when nominal strain is 2.0%;
14 SD10 and SD40 models with RD-split texture and an SD40 model with basal
15 texture with high strain rates on slip strains; (a) AS condition and (b) BP condition.
- 16
- 17 Table 1 Texture types and the orientation of their (0001) axis
- 18 Table 2 Elastic compliance of pure titanium [(TPa)⁻¹] [31]

1 Table 3 Values used for the Voce equation [MPa]

2 Table 4 Conditions of strain rate sensitivity m [16,17]

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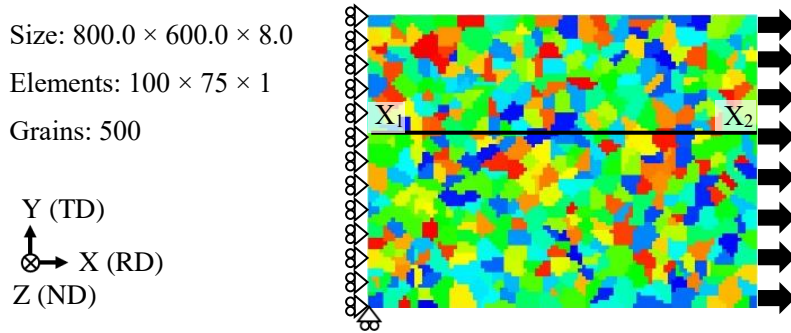
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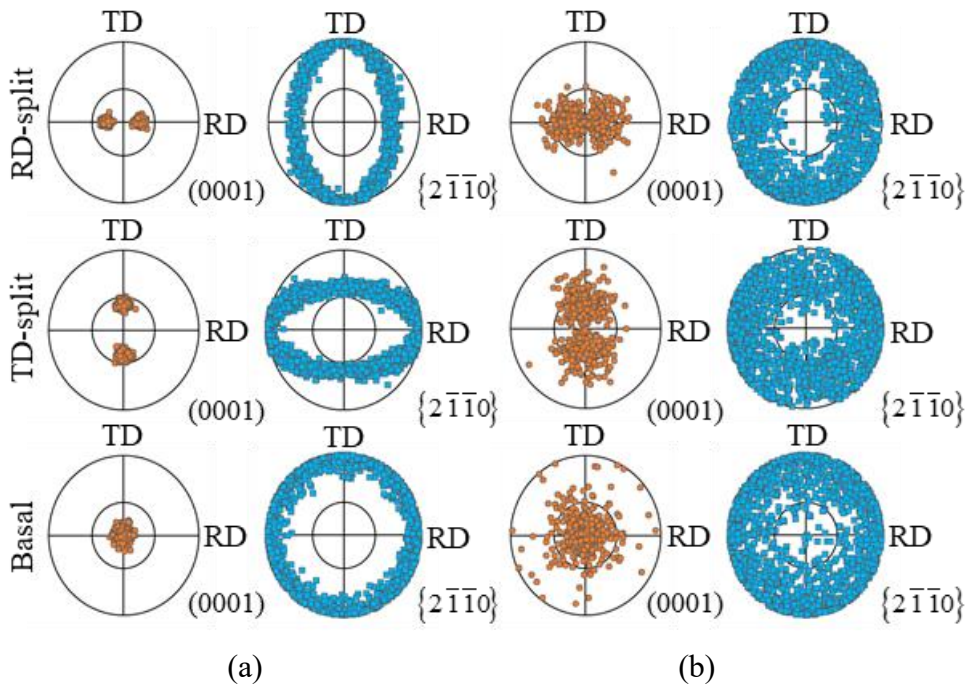
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17 **Figures**



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Fig. 1 Polycrystalline model of α -Ti.



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Fig. 2 Pole figures of (a) SD10 model and (b) SD40 model with RD-split, TD-split, and basal textures.

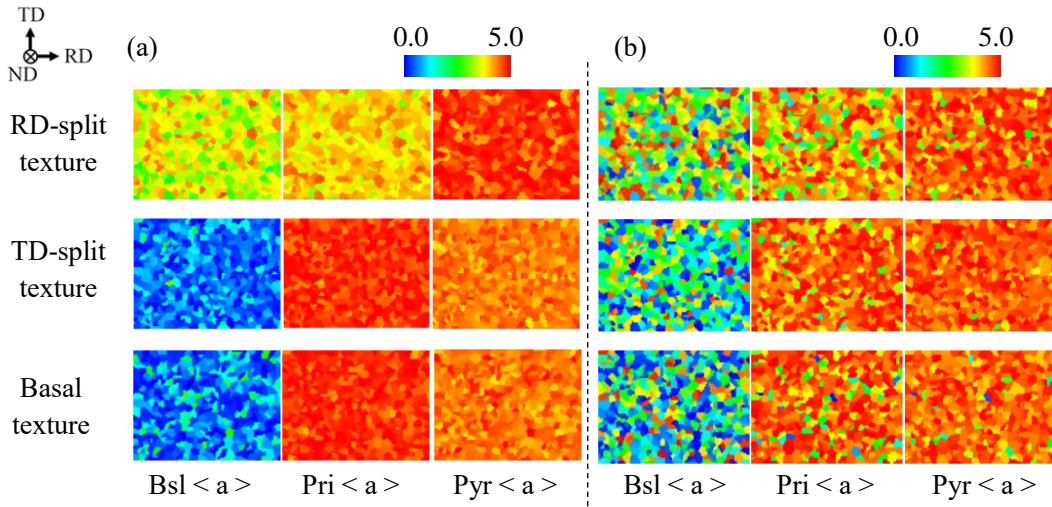


Fig. 3 Distributions of Schmid factors in (a) SD10 and (b) SD40 models.

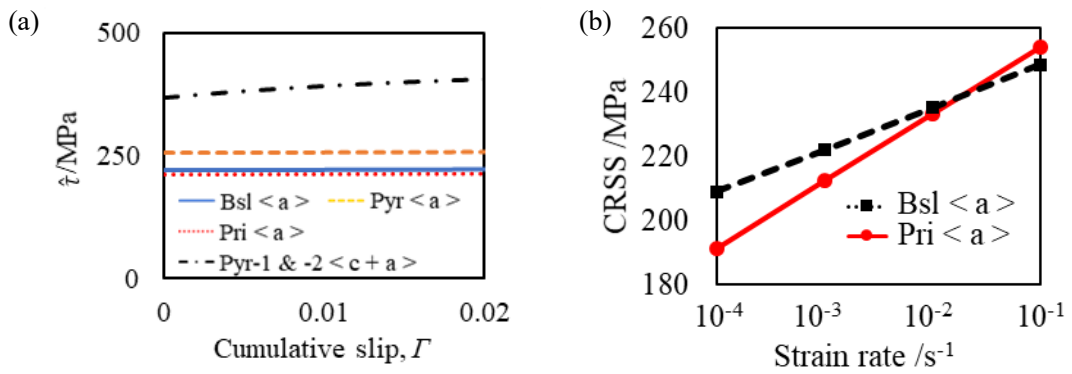
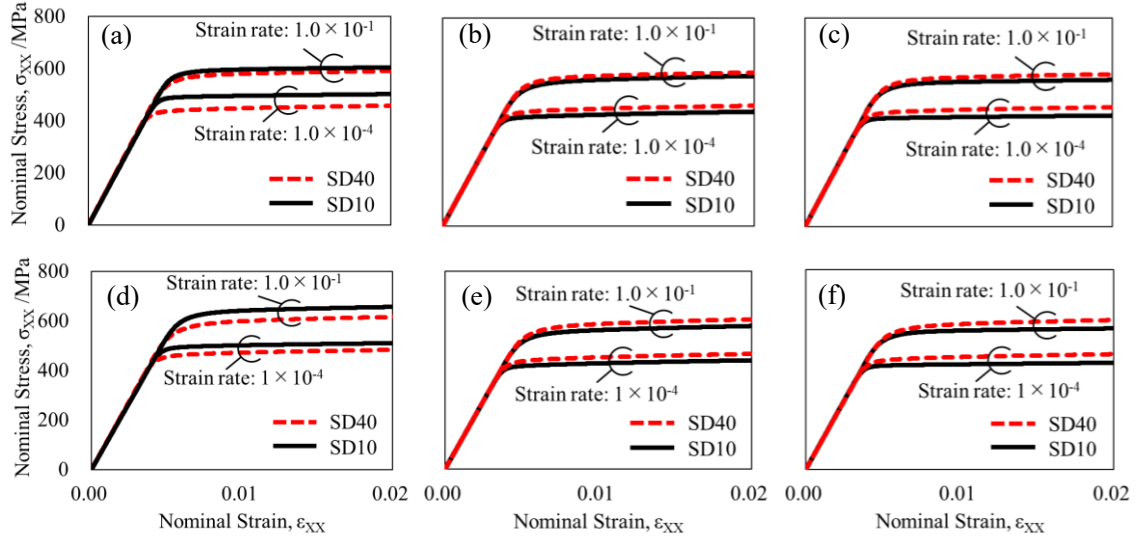


Fig. 4 (a) $\hat{\tau}$ for each slip system as a function of cumulative slip strain and (b) initial

CRSSs for Bsl $\langle a \rangle$ and Pri $\langle a \rangle$ depending on the strain rates [18].

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3 Fig. 5 Profiles showing the relationship between nominal stress and strain obtained by

4 models with RD-split texture (a, d), TD-split texture (b, e), and basal texture (c, f).

5 Activation of Pyr < a > is considered in (a–c) and not considered in (d–f).

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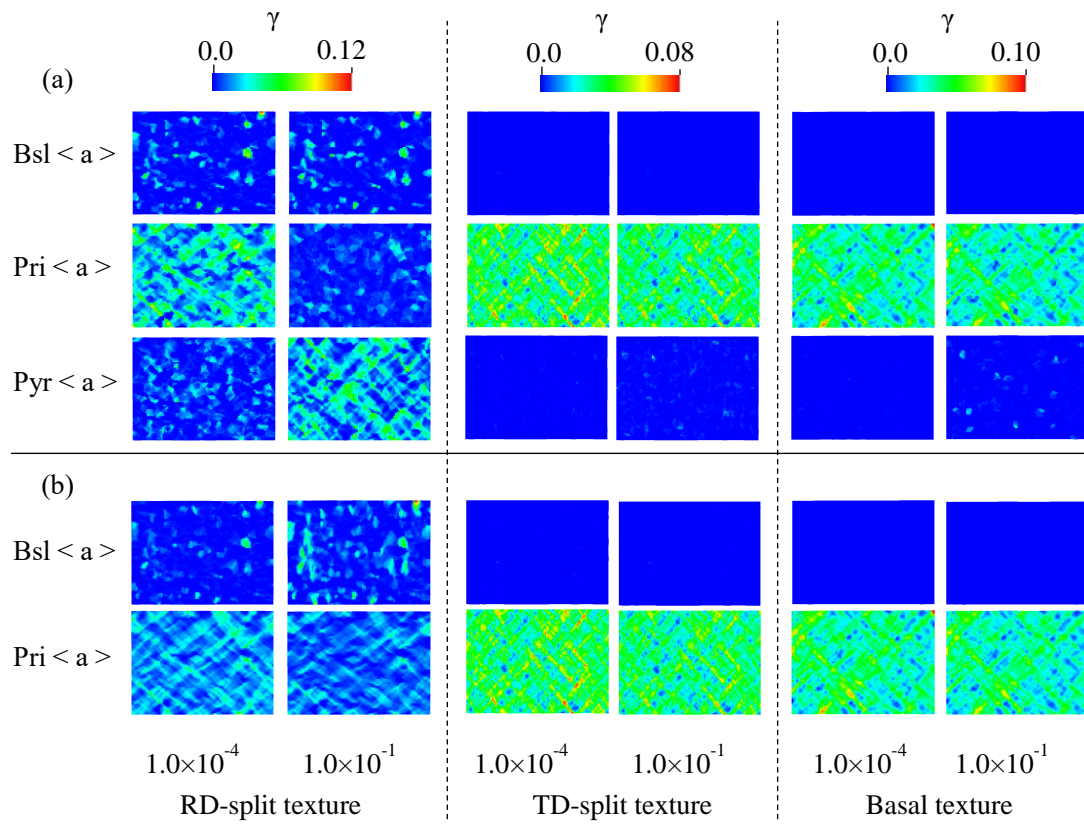
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2 Fig. 6 Slip strain distributions when SD10 models are employed, and nominal strain is

3 2.0 %; (a) AS condition and (b) BP condition.

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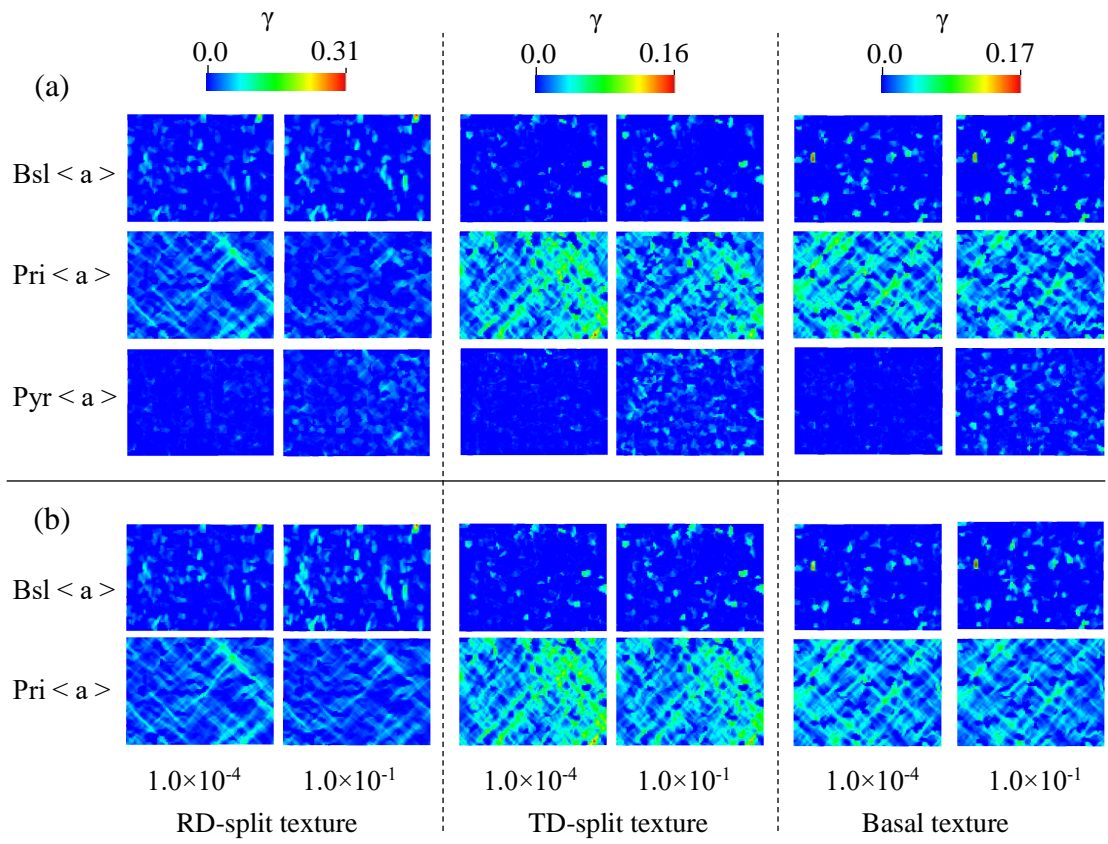
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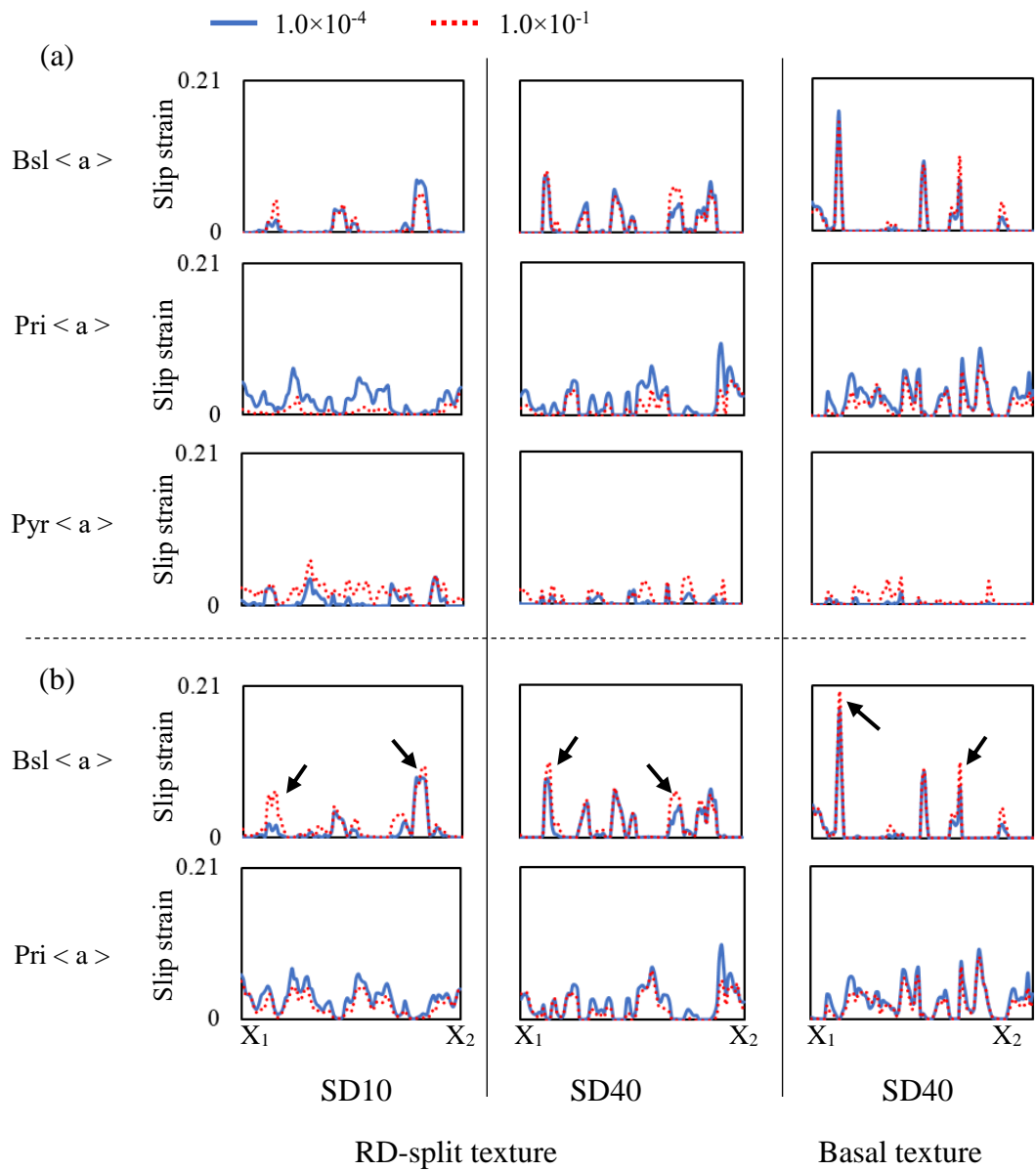
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Fig. 7 Slip strain distributions when SD40 models are employed and nominal strain is 2.0 %; (a) AS condition and (b) BP condition.



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2 Fig. 8 Line profiles of slip strain along X_1 – X_2 in Fig. 1 when nominal strain is 2.0%;

3 SD10 and SD40 models with RD-split texture and an SD40 model with basal texture with

4 high strain rates on slip strains; (a) AS condition and (b) BP condition.

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1 Tables

2 Table 1 Texture types and the orientation of their (0001) axis

Texture types	Orientation of (0001) axis
RD-split	20°–30° inclination from ND to RD
TD-split	30°–40° inclination from ND to TD
Basal	Parallel to ND
T (Transverse)	Parallel to TD
R (RD)	Parallel to RD

3

4 Table 2 Elastic compliance of pure titanium [(TPa)⁻¹] [31]

S_{11}	S_{12}	S_{13}	S_{33}	S_{44}
9.581	-4.623	-1.893	6.983	21.413

5

6 Table 3 Values used for the Voce equation [MPa]

Slip systems		τ_0	τ_1	θ_0	θ_1
Bsl < a >		220	400	100	200
Pri < a >		210	400	100	200
Pyr-1 < a >	AS condition	255	400	100	200
	PB condition	Inactive			
Pyr-1 < c + a > and	AS condition	369	50	3000	100
Pyr-2 < c + a >	PB condition	Inactive			

7

8 Table 4 Table 4 Conditions of strain rate sensitivity m [16,17]

Bsl < a >	Pri < a >	Pyr-1 < a >	Pyr-1 < c + a > and Pyr-2 < c + a >
0.025	0.041	0.020	0.020

