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To cite this article: Huigang Shi, Jianye Chen, Junqiang Lu, Libing Zhu, Lefu Zhang, Jiuxiao Li, Weijie Lu & Xianglong Guo (2024) The activation of multiple slip systems in polycrystalline zirconium by using automated lattice rotation framework, Materials Research Letters, 12:12, 912-920, DOI: [10.1080/21663831.2024.2402370](https://doi.org/10.1080/21663831.2024.2402370)

To link to this article: <https://doi.org/10.1080/21663831.2024.2402370>



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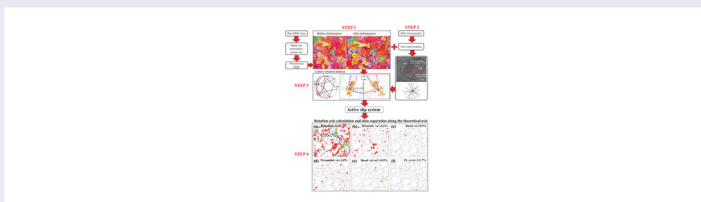
The activation of multiple slip systems in polycrystalline zirconium by using automated lattice rotation framework

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ABSTRACT

Understanding the deformation mechanism in polycrystalline metals is critical to use them in high-value high-risk applications. Here, we report an automated framework based on lattice rotation analysis for accurately identifying slip system and assessing the multiple slip activities in large data set of polycrystalline Zr, aims to statistically provide deep insight on deformation mechanism of Zr. Results show that multiple slip is the dominant slip system rather than single slip system. This method can be applied as a complementary method to the intragranular misorientation axis (IGMA) method and can act as bridges between macro-mechanical response and microstructural deformation mechanisms.



ARTICLE HISTORY

Received 21 February 2024

KEYWORDS

Zirconium; plastic deformation; polycrystals; lattice rotation; multiple slip

Introduction

Zirconium alloys have been widely used as fuel rod cladding and structural fuel assembly components due to an attractive combination of adequate corrosion resistance, favorable mechanical properties and relatively low neutron capture cross-section [1–3]. Thermo-mechanical treatments of these components for engineering application frequently involve a series of deformation processes, such as hot/cold rolling, extrusion and forging [4,5]. In addition, these components are inevitably subjected to environmental stress/strain during long-term service [6–8], thereby causing continuous deformation. For instance, the plastic deformation caused by fretting wear can frequently take place in the fuel assembly grid due to the flow-induced vibrations [6,7]. Meanwhile, the pellet-cladding mechanical interaction would inevitably give rise to strain deformation

in the cladding tubes, particularly under high burn-up conditions [8]. This strain deformation may often have adverse impact on the service behavior of cladding tubes, particularly on the performance of fretting corrosion behavior, which has emerged as the most serious failure mode in recent years [9]. According to the International Atomic Energy Agency (IAEA) [10], ~58% of failures of cladding tubes were attributed to fretting deformation and corrosion in the year of 2011–2015, posing a significant threat to the safe operation of nuclear reactors. Thus a comprehensive knowledge about the deformation mechanisms in zirconium alloys is of prime importance, especially during forming of the cladding tubes and during reactor operating conditions.

With respect to the plastic deformation of hexagonal close-packed (HCP) α -Zr metals, extensive effort has been directed toward deconvoluting the slip and

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Supplemental data for this article can be accessed online at <https://doi.org/10.1080/21663831.2024.2402370>.

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twinning mechanisms, as has been thoroughly documented in review articles [11–14]. Recent experimental observations have proved that the multiple slip system in polycrystalline Zr can be activated at room temperature [15]. *In-situ* neutron diffraction measurements of Zr during compression also confirms the activation of various slip modes [16], and cross-slip events between prismatic and basal slip have been visualized using *in-situ* TEM at ambient temperature [17]. Despite these works, the multiple slip systems responsible for the accommodation of strain imposed on polycrystalline Zr have not yet been fully described. The dilemma is between precisely identifying the active slip systems while sampling a statistically valid number of grains, especially at large strains. To date, surface trace analysis is the most commonly used method to uncover the active slip modes and its kernel lies in the comparison of observed slip trace on the crystal surface with the theoretical one [18]. Recently works by Zeng et al. [19,20] systematically investigate the cyclic deformation mechanism of zirconium at micro-scale (grain/sub-grain scale) by using EBSD-assisted slip trace analysis. However, this method is useless when there are two or more possible slip systems in a given slip plane with identical slip traces [21]. Apart from this, the Burgers vector determination strategy based on transmission electron microscopy (TEM) allows for identification of active slip systems in deformed polycrystals [22,23], but is considerably time-consuming to analyze a sufficient number of grains, and this approach is limited to materials deformed to a small strain. More recently, high-resolution digital image correlation (HRDIC) is becoming a prominent technique for investigating deformation behavior at grain scale, which provides high-precision and quantitative local strain maps of surface deformation [24], and is commonly used in conjunction with electron backscatter diffraction (EBSD) to correlate grain orientation with strains and slip system activity [25]. In particular, the relative displacement ratio (RDR) technique using HRDIC is a powerful method to accurately determine the active slip system in metallic alloys [26]. By analyzing the relative displacements of microstructural features on the surface of samples subjected to external loading, this technique enables us to identify the specific slip systems that are activated during plastic deformation with a high degree of precision [27,28]. Unfortunately, there are some potential disadvantages associated with this method, such as computational complexity, sensitivity to noise and artifacts, and calibration challenges [29]. The analysis of high-resolution digital images to calculate the relative displacement ratio requires sophisticated image processing algorithms and can be resource-intensive in terms of both computational power and time, thereby restraining the widespread application of this method.

In this case, it is necessary to develop other criteria or methods to identify the active slip systems for a large number of grains in polycrystals, aiming to draw accurate conclusions on the deformation mechanism.

Recently, the intragranular misorientation axis (IGMA) analysis proposed by Chun et al. [30] has been widely used to identify the activated slip systems. This approach is a powerful tool to investigate the slip nature by slip-induced lattice rotation since it can be performed on a large sample scale and has been utilized to analyze the deformation behavior in hcp metals such as Ti, Mg and Zr alloys [31–33]. However, the active slip system cannot be identified by this method if there is one rotation axis being shared by multiple slip modes, such as basal $\langle a \rangle$ and second pyramidal $\langle c+a \rangle$ slip [34]. Furthermore, plastic deformation studied by IGMA analysis was still confined to single dominant slip system rather than multiple slip modes being discussed to date. In this case, other techniques, such as slip trace-modified lattice rotation analysis (ST-MLRA) were proposed by Yang et al. [35,36] before, after considering both slip plane and lattice rotation information. The slip plane trace orientation is used to define the potential active slip planes while the actual slip direction within the active slip plane is obtained from the grain rotation, as indicated by the stretching of the trace of the grain orientation in the pole figure as a result of deformation. They showed that the strategy is simple to implement and allows to accurately identify the active slip system in each grain. However, a large-field analysis involving hundreds or even thousands of grains will be labor-and-time-consuming if experimental slip trace angles are measured on a grain-by-grain basis.

To perform a large-field slip trace analysis with high-precision and investigate the multi-slip intrinsic deformation mechanism of polycrystalline metals in an automated and time-saving fashion, we proposed an automated framework based on the ST-MLRA method for accurately identifying slip system and assessing the multiple slip activities in large data set of polycrystalline Zr. This optimized method can provide advantages to identify all the triggered slip systems and statistically present the relative activities of all slip modes. With assistance of this method, some attempts were made to uncover the underlying deformation mechanisms of polycrystalline Zr, which can offer new insight toward development of high-performance Zr alloys.

Materials and methods

The nominal chemical compositions of the experimental alloy used here were 0.5 wt.% Sn, 0.4 wt.% Nb, 0.3 wt.% Fe, 0.05 wt.% Cu and balanced Zr. The alloy was prepared by a sequence of three times vacuum arc re-melting,

a hot forging at 1000°C, a β -quenching at 1050°C for 0.5 h, a hot rolling at 650°C and four times of cold rolling followed by annealing at 550°C for 4 h. Dog-bone shaped tensile samples with 16 mm gauge size, 4.0 mm width and 0.6 mm thickness were machined respectively along the rolling direction (RD) and transverse direction (TD). Then room temperature tensile tests were conducted at strain rates of $1.0 \times 10^{-4} \text{ s}^{-1}$ using a universal testing machine (Roell, Z020, Zwick) equipped with an electronic extensometer. At least three samples were tested to guarantee repeatability under each condition and representative curves were displayed. Interrupted microstructural characterization was performed successively at engineering strains of $\sim 5\%$, $\sim 10\%$ and $\sim 15\%$, by using *quasi-in-situ* electron backscatter diffraction (EBSD, Tescan, Mira-3) system, and the EBSD data was recorded using an Oxford Symmetry2 camera with a working distance of 17 mm, acceleration voltage of 20 keV, and current of $\sim 7.8 \text{ nA}$. All crystallographic and slip systems data manipulation for large data set of EBSD was performed using an in-house Matlab program in the MTEX toolbox [37]. The detailed steps of the automated framework utilized in this work can be found in the Supplementary Materials.

Results and discussion

As displayed in Figure 1(a), the EBSD inverse pole figure (IPF) illustrates that the sample after annealing exhibits a fully recrystallized microstructure with well-equiaxed α -Zr grains, and the average grain size is $\sim 4.5 \mu\text{m}$. The associated 0001 pole figure (Figure 1b) indicates that the sample possesses a strong basal texture, manifesting as basal pole deviating $0\text{--}30^\circ$ away from the normal direction (ND) (red colored grains). Figure 1(c) exhibits the engineering stress–strain curves of sample tested along RD and TD at strain rate of 1×10^{-4} . The nomenclature of samples herein is the following: RD and TD denote tensile deformation along RD and TD, respectively, and they are following by the plastic strain level (e.g. ‘RD-5 %’ stands for ‘specimen deformed along RD up to 5 %’). Remarkably, TD sample demonstrates a relatively higher yield strength (YS, $396 \pm 4 \text{ MPa}$) than RD sample ($363 \pm 9 \text{ MPa}$), indicative of yielding anisotropy in our alloy. These anisotropic yielding behaviors of our materials and the following anisotropic mechanical performance can be occurred with the preferred slip system, which will be discussed in the following paragraphs. Moreover, a characteristic yield drop at the initial stage of plastic deformation is observed (inset of Figure 1c), and this phenomenon can be interpreted in terms of the shortage of mobile dislocations in our previous work [38]. After yielding, the flow stress climbs rapidly for

RD sample and gradually exceeds the stress value of TD sample after $\sim 3\%$ strain. Consequently, the difference between ultimate tensile strength (UTS) and YS (UTS-YS, $\sim 95 \text{ MPa}$), as well as the total elongation (El, $\sim 32\%$) for RD sample are both prominently higher than that for TD sample ($\sim 25 \text{ MPa}$ and $\sim 29\%$, respectively), indicative of a relatively higher work-hardening capability along RD (Figure 1d).

Figure 2 exhibits an example to identify the active slip modes in grain G1 ($\sim 4.8 \mu\text{m}$) with average Euler angles of (166.8° , 18.3° , 236.7°) by using the automated framework based on the ST-MLRA method. The IPF maps of G1 before and after deformation in Figure 2(a) reveal that G1 has been apparently elongated along RD and the local orientation has been slightly changed due to dislocation slip after RD-10 % strain, as the color contrasts inside grain is not uniform. The corresponding scanning electron microscope (SEM) image shows that several planar slip systems have been triggered after 10% strain, and two types of slip traces are observed (marked as the red and blue dashed lines in Figure 2b). Further slip trace analysis (Figure 2c) demonstrates that the experimental slip traces are compatible with two possible active slip systems: $(\bar{1}100)[\bar{1}\bar{1}20]$ prismatic $\langle a \rangle$ (No. 5, $m = 0.489$) and $(11\bar{2}2)[11\bar{2}\bar{3}]$ pyramidal II $\langle c+a \rangle$ (No. 18, $m = 0.385$). Figures 2(d and e) respectively depict the experimental projection of the orientation of G1 before and after deformation in 0001 and $\{10\bar{1}0\}$ pole figures. It is noted that slip deformation stretches the projection along some specific directions (see the magenta scatters in the enlarged portion of Figures 2d and e), indicative of lattice rotation of G1. Moreover, the spread directions agree well with the theoretical predictions corresponding to lattice rotation axis (RA)- $[1\bar{N}00]$ (Figure 2d-1, the green arrow of C) and RA- $[0001]$ (Figures 2e-1 and e-2, the purple arrow of D). Thus it is reasonable to conclude that the lattice of G1 has rotated around $[0001]$ and $[1\bar{N}00]$ axes, respectively. According to IMGA analysis [30], prismatic $\langle a \rangle$ and pyramidal II $\langle c+a \rangle$ dislocation activities will result in lattice rotation around $[1000]$ and $[1\bar{N}00]$ axes, respectively. The local slip deformation in G1 is therefore suspected to be induced by the prismatic $\langle a \rangle$ and pyramidal II $\langle c+a \rangle$ dislocation activity, which shows the best match with the experimental slip traces in G1.

Furthermore, the locations of activated prismatic $\langle a \rangle$ and pyramidal II $\langle c+a \rangle$ slip in G1 can be respectively colored according to the triangle of rotation axis in Figure 2(f). It is noted that prismatic $\langle a \rangle$ slip has been triggered in the right part and close to the grain boundaries (GB) of G1, dominating an area fraction of $\sim 23.1\%$ (colored as red in Figure 2f). Pyramidal II $\langle c+a \rangle$ slip, however, is activated at the top left corner

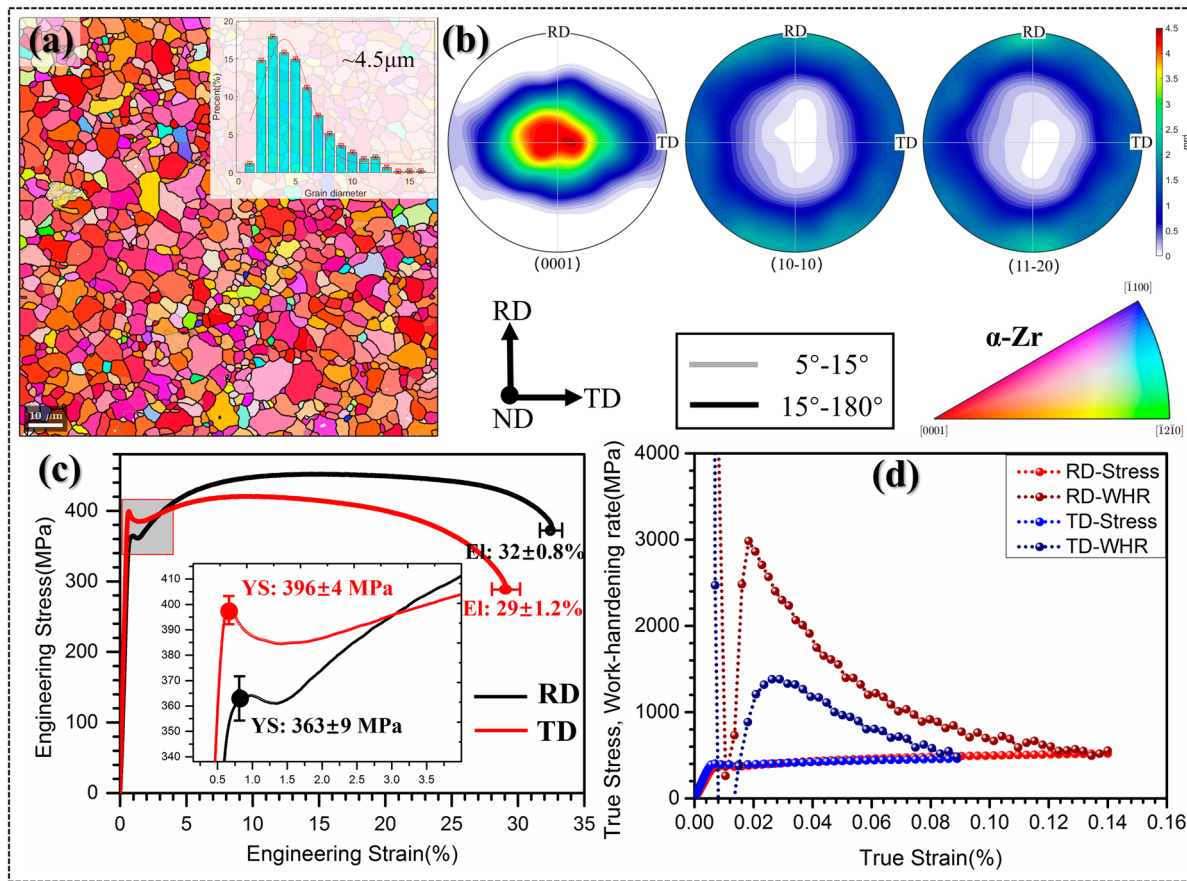


Figure 1. (a,b) EBSD inverse pole figure (IPF) and the pole figures of sample, respectively; (c) engineering stress versus engineering strain curves; (d) work-hardening rate (WHR) versus true strain curves for RD sample and TD sample, respectively.

of G1, accounting for only $\sim 8.2\%$ area fraction (colored as blue in Figure 2f). The detailed information about the definition of area fraction of each slip system and how to calculate it from the raw EBSD data can be found in the Supplementary Materials (Figure S3). This result is very interesting because the experimental slip activities of G1 (Figure 2b, the SEM image) match well with the misorientation axes map (Figure 2f) predicted by the modified lattice rotation analysis. Thus the dominant slip system in grain G1 is $(\bar{1}100)[\bar{1}\bar{1}20]$ with a macroscopic Schmid factor of 0.489, and $(11\bar{2}2)[11\bar{2}3]$ pyramidal II $\langle c+a \rangle$ slip can also be activated despite of its higher critical resolved shear stress (CRSS) [39]. The activation of pyramidal II $\langle c+a \rangle$ slip can be interpreted as local strain concentration caused by grain neighboring effect with heterogeneous slip [40] (see Figure S3d in Supplementary Materials).

A more complex scenario is found in a relatively large grain G2 ($\sim 17.2\ \mu\text{m}$) with average Euler angles (85.5° , 167.4° , 198.3°) after the same RD-10 % strain. As displayed in Figure 3(a), the orientation non-uniformity of G2 is more evident compared with G1, suggesting that G2 possesses higher plastic strain than G1. The

slip trace analysis in G2 shows that the best match between the experimental and theoretical traces is found for $(\bar{1}100)[\bar{1}\bar{1}20]$ prismatic $\langle a \rangle$ (red dashed line, No. 5, $m = 0.46$) and $(\bar{1}01\bar{1})[\bar{1}\bar{1}20]$ pyramidal $\langle a \rangle$ (pink dashed line, No. 9, $m = 0.49$). However, some curved slip lines can be observed in the SEM image of G2 (orange lines), which obviously connect with either prismatic $\langle a \rangle$ or pyramidal $\langle a \rangle$ slip line. These curved lines are not belonged to any slip system predicted by the standard slip trace analysis due to the relatively large deviation angle between experimental and predicted trace line ($> 10^\circ$). Figure 3(d) exhibits the orientation of G2 on the $\{10\bar{1}0\}$ pole figure which, before and after deformation, is plotted by numerous scattered points that illustrate the deformation-induced lattice rotations in individual grain. It is apparent from the enlarged views (d-1 and d-2) that the stretching direction of G2 is compatible well with theoretical predictions with respect to the rotation axes $[0001]$ (purple arrow of D) and $[10\bar{1}2]$ (magenta arrow of E). Consequently, dislocation slip within G2 preferentially occurs on the $(\bar{1}100)$ prismatic plane along $[\bar{1}\bar{1}20]$ direction and $(\bar{1}01\bar{1})$ pyramidal plane along $[\bar{1}\bar{1}20]$ direction. Moreover, the locations of these

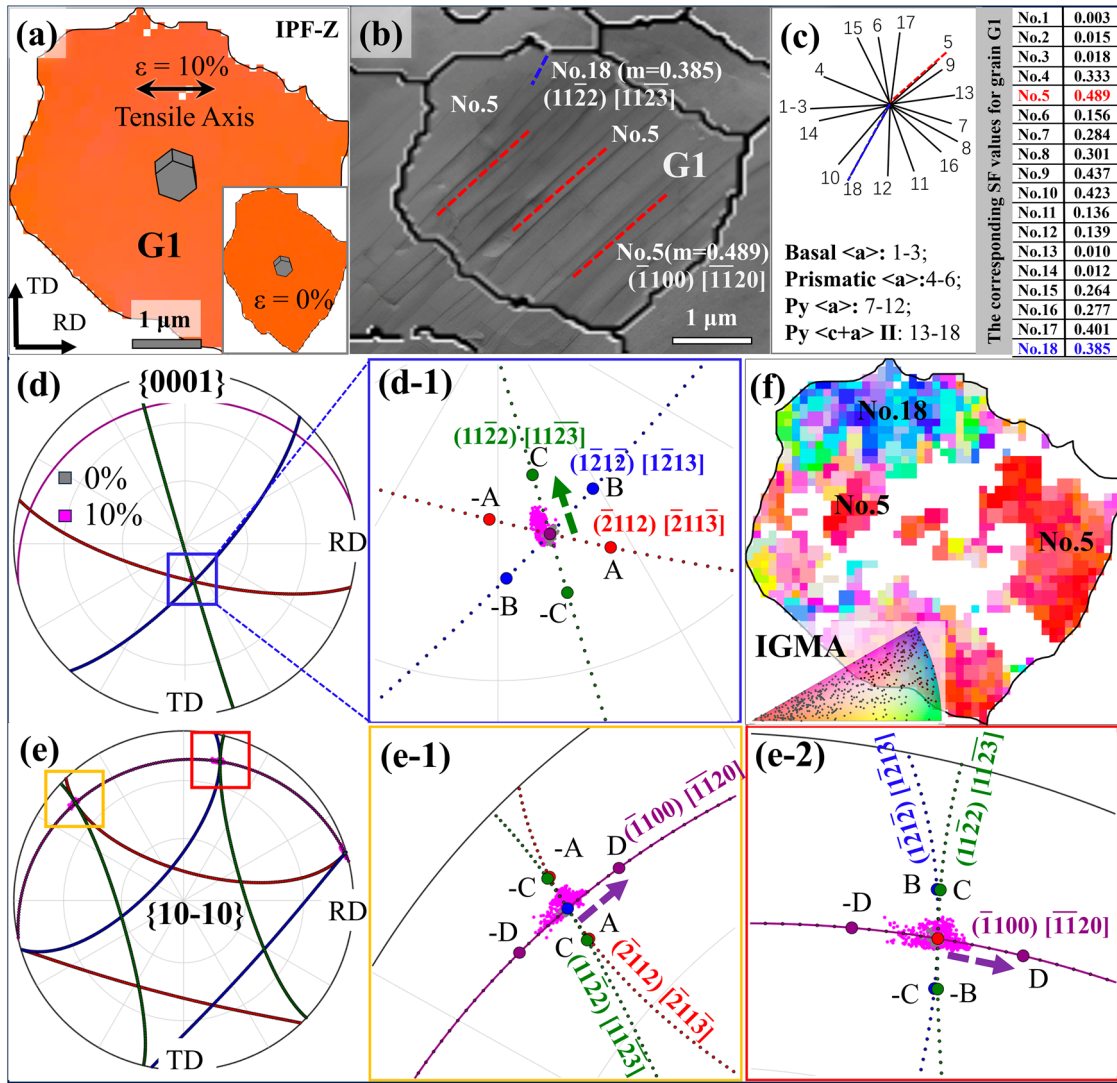


Figure 2. (a) EBSD inverse pole figure (IPF) map providing orientation information of G1 after tensile deformation up to 10 %, with average Euler angles (166.8° , 18.3° , 236.7°). The EBSD IPF map before deformation of G1 was also included; (b) Scanning Electron Microscope (SEM) image of G1 after tensile deformation up to 10 %; (c) the EBSD-assisted slip trace analysis of G1, and the corresponding Schmid factor (SF); (d,e) projection of G1 before and after deformation on the 0001 and $\{10\bar{1}0\}$ pole figure, respectively. The circular lines stand for the theoretical predictions in orientation due to the lattice rotation along both prismatic $\langle a \rangle$ and pyramidal II $\langle c+a \rangle$ slip systems, and in which the dots correspond to a rotation of $\pm 5^\circ$; (f) the misorientation axis map for G1. The in-grain misorientation axis (IGMA) distribution maps for G1 with hexagonal symmetry was also included.

activated slip systems (Figure 3b) are essentially consistent with the misorientation axes map of Figure 3(e) (e.g. prismatic $\langle a \rangle$ slip dominating at the lower right corner of G2 and pyramidal $\langle a \rangle$ slip locating at the upper left corner, respectively). It is noted that the curved slip occurs at the position colored by yellow or green within G2 (black circle in Figure 3e), and neither prismatic nor pyramidal $\langle a \rangle$ slip belongs to. Two possible reasons can be included, as follows: first, it is associated with the simultaneous operation of prismatic $\langle a \rangle$ and pyramidal $\langle a \rangle$ slip, indicating that multiple slip plays a significant role to accommodate plastic deformation

[41]; on the other hand, the distribution of misorientation angle within grains is usually non-uniform in many cases [42], as evidenced by the in-plane lattice rotation angle around the sample coordinate axis of Z (Figure 3f). Clearly, opposite lattice rotations can be observed in the left (clockwise rotation) and right regions (anti-clockwise rotation) of the grain G2. Thus curved slip lines will be evolved from straight line due to the slip-induced lattice rotation along opposite directions for the left and right regions of G2.

To further unveil the quantitative activities of various slip modes, statistical analysis of approx. 500 grains were

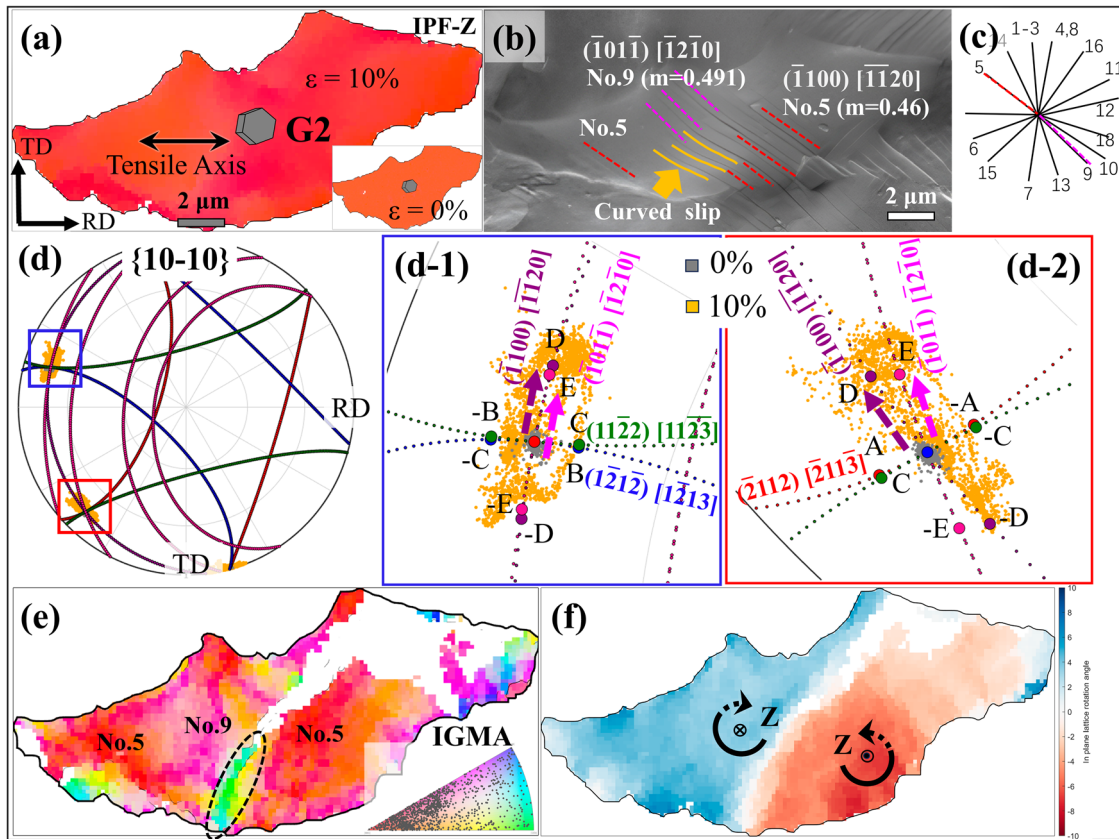


Figure 3. (a) IPF map of G2 after tensile deformation up to 10 %, with average Euler angles (85.5°, 167.4°, 198.3°); (b) SEM image of G2 after tensile deformation up to 10 %; (c) the EBSD-assisted slip trace analysis of G2; (d) projection of G2 before and after deformation on the {10 $\bar{1}$ 0} pole figure. The circular lines stand for the theoretical variation in orientation due to the lattice rotation along both prismatic and pyramidal $\langle a \rangle$ slip systems, and in which the dots correspond to a rotation of $\pm 5^\circ$; (e) the misorientation axis map and in-grain misorientation axis (IGMA) distribution maps for G2; (f) in-plane lattice rotation angle around the principal direction Z//ND for G2.

conducted by using this automated slip system identification framework on the raw EBSD data of polycrystalline Zr after tension of 5 %, 10 % and 15 % strains. Note that grains containing multiple sub-grains have been excluded at the beginning of analysis to improve the reliability of data. According to previous literature [43,44], grain orientation spread (GOS) refers to the average of the misorientation angle to the grain-mean orientation and has been widely used to distinguish the recrystallized grains from deformed grains. Thus recrystallized grains with a GOS value less than 1° (as shown in Figure S2) have been extracted and analyzed by using the modified lattice rotation analysis. As shown in Figure 4, three significant features are observed from this set of tensile deformations. The first finding is that the area fraction of each slip system progressively increases with the progress of deformation, regardless of RD or TD specimens, indicative of more dislocation activities with accumulative tensile strain in polycrystalline Zr. The second finding is that multi-slip is the dominant slip mode and prismatic $\langle a \rangle$ plays a second role, followed by pyramidal $\langle a \rangle$ and first pyramidal $\langle c+a \rangle$ slip in the whole deformation,

especially at large strains. The last discovery is that RD sample possesses relatively higher fraction of multiple slip and/or prismatic $\langle a \rangle$ systems, as well as stronger pyramidal $\langle a \rangle$ activity within grains than that of TD sample, particularly at large strains (highlighted in bold in Table 1).

As is well known, the interaction between dislocations and GB or low-angle GB on different slip systems plays an essential role in controlling the mechanical properties of polycrystalline metals [45]. At the onset of deformation ($\sim 1\%$), the anisotropic yielding behavior of our sample is experimentally observed (Figure 1c), and this feature has been well elucidated from the viewpoint of grain orientations and normalized SF in our previous work [46]. After yielding (e. g. $\sim 5\%$ strain), the most favorable slip mode is the multiple slip, and the area fraction of each slip is relatively higher for RD sample than TD sample (e.g. $\sim 3.6\%$ fraction of prismatic $\langle a \rangle$ slip for RD sample versus $\sim 3.1\%$ fraction of prismatic $\langle a \rangle$ slip for TD sample). It is therefore reasonable to conclude that for RD sample, more grains are favorable to slip than TD sample, thereby causing a higher

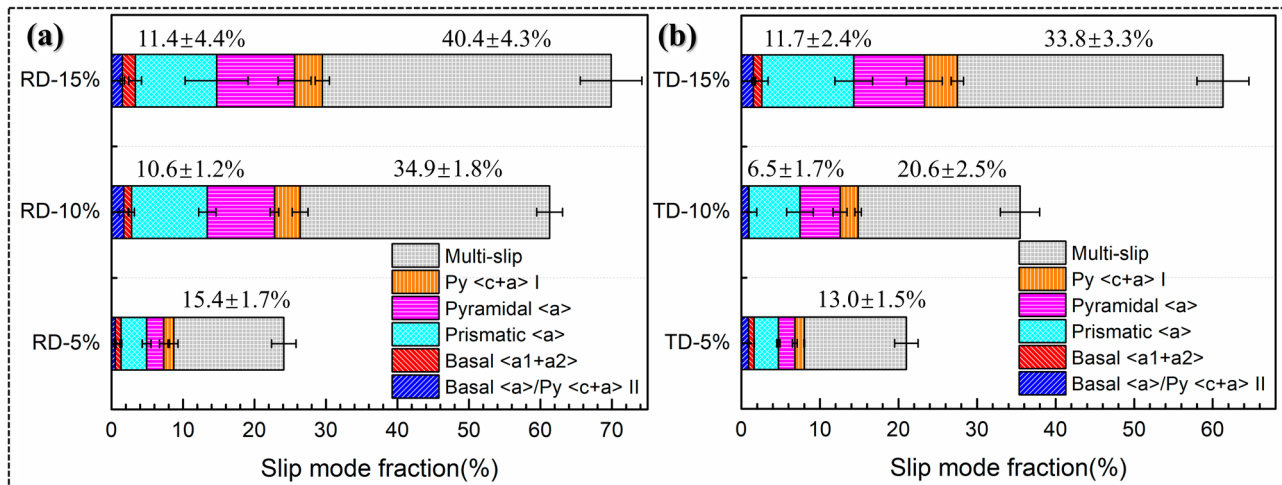


Figure 4. Summary of the area fraction of various slip systems activated in (a) RD sample and (b) TD sample at different strains.

Table 1. Statistical data of slip systems measured by modified lattice rotation analysis.

Alloys	Area fraction of different slip systems (%)					
	Basal < a > /Py < c+a > II	Basal < a ₁ +a ₂ >	Prismatic < a >	Pyramidal < a >	Py < c+a > I	Multiple slip
RD-5 %	0.5 ± 0.1	0.8 ± 0.1	3.6 ± 0.6	2.4 ± 0.6	1.4 ± 0.6	15.4 ± 1.7
RD-10 %	1.7 ± 0.6	1.1 ± 0.4	10.6 ± 1.2	9.4 ± 0.6	3.6 ± 1.1	34.9 ± 1.8
RD-15 %	1.5 ± 0.3	1.8 ± 0.9	11.4 ± 4.4	10.9 ± 2.3	3.9 ± 1.0	40.4 ± 4.3
TD-5 %	0.9 ± 0.05	0.7 ± 0.03	3.1 ± 0.2	2.1 ± 0.3	1.2 ± 0.04	13.0 ± 1.5
TD-10 %	0.9 ± 0.03	1.0 ± 0.06	6.5 ± 1.7	5.1 ± 0.9	2.3 ± 0.4	20.6 ± 2.5
TD-15 %	1.5 ± 0.2	1.1 ± 0.8	11.7 ± 2.4	9.0 ± 2.3	4.2 ± 0.8	33.8 ± 3.3

work-hardening capacity. The dislocation slip is partly restricted at the early stage of deformation along TD, resulting in a lower strain hardening capability. As the strain progressed, interactions between dislocations on multiple slip systems can therefore form dislocation barriers, which block further dislocation gliding and thus lead to further strain hardening. At large strains (e. g. $\sim 10\%$ or 15%), the higher frequency of multiple slip and prismatic $\langle a \rangle$ slip activities, as well as stronger pyramidal $\langle a \rangle$ activity within grains is obtained in RD sample. It is well known that the activation of multiple slip system is commonly correlated with excellent dislocation pile-up or storage capabilities [47], and pyramidal $\langle a \rangle$ slip is difficult to be triggered except for conditions with large local stress, due to its higher CRSS [48,49]. The prevalence of pyramidal $\langle a \rangle$ slip could be interpreted as prismatic $\langle a \rangle$ screw dislocations cross-slipping on first-order pyramidal planes due to a non-planar dislocation core structure which dissociates into two partial dislocations [50]. Thus it is reasonable to infer that multiple slip, prismatic $\langle a \rangle$ and pyramidal $\langle a \rangle$ slip is greatly facilitated in RD sample with large strain, contributing to the enhancement of work-hardening capacity. In this case, RD sample would exhibit better tensile strength–ductility synergy than TD sample, leading to prominent mechanical anisotropy in late deformation.

Conclusion

In summary, an automated framework based on the modified lattice rotation analysis has been proposed and demonstrated to precisely identify the active slip system by large-field EBSD data containing a large number of grains. The anisotropic deformation accompanying with multiple slip activities has been quantitatively investigated in a polycrystalline zirconium alloy. Our results suggest that various slip systems are locally active in different regions of grains, and the most dominant slip system is the multiple slip, followed by prismatic $\langle a \rangle$ slip in the whole deformation. The stronger activities of multiple slip, prismatic $\langle a \rangle$ and pyramidal $\langle a \rangle$ slip are essentially presumed to be responsible for the better work-hardening capability in RD sample. The combination of this automated slipping system identification framework and IGMA is anticipated to enhance our understanding of the fundamental deformation mechanisms of polycrystals.

Disclosure statement

No potential conflict of interest was reported by the author(s).

Funding

This work was financially supported by the National Natural Science Foundation of China (grant number 52201081).

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