

# Twinning behavior of polycrystalline alpha-uranium under quasi static compression



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## ARTICLE INFO

### Article history:

Received 25 November 2015

Received in revised form

28 May 2016

Accepted 30 May 2016

Available online 1 June 2016

### Keywords:

Uranium

Deformation twin

Quasi static compression

Electron backscattered diffraction

Transmission electron microscopy

## ABSTRACT

Deformation twins in cast uranium strained to 4.2% and 6.2% by quasi static compression were investigated using electron backscattered diffraction and transmission electron microscopy. Twin types of {130}, {172}, {112} and {176} were observed in present experiment. All the operative twin variants in each twin type have the highest Schmid factor among the equivalent variants. Some {130} twins in cast uranium were inclined to disappear during subsequent loading through the re-twinning processes with Schmid factor values greater than 0.4. The ‘(−176)’ variant was identified by indexing the electron diffraction pattern combining with the stereographic projection analysis. Twin pairs of ‘(−176)’ – ‘(−17−2)’ occurred in the adjacent grains were well matched with the geometric compatibility factor value of 0.933.

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## 1. Introduction

Twinning plays an important role in the plastic deformation modes of polycrystalline  $\alpha$ -uranium ( $\alpha$ -U) which has a low crystal symmetry of base-centered orthorhombic (BCO) [1,2]. Uranium is the only metal which exhibits twins of Type I, Type II, and compound. Type I twins have rational Miller indices in  $K_1$  and  $\eta_2$  elements, type II twins have rational  $K_2$  and  $\eta_1$ , and compound twins have all four twinning elements being rational.

Cast uranium usually contains a significant amount of twins resulted from inter-granular stresses that induced by volume shrinkage of  $\gamma \rightarrow \beta \rightarrow \alpha$  phase transformation [3] and anisotropic thermal expansion [4–6] during cooling. However, researches on the evolution of twins in cast uranium during subsequent loading are limited. In some metals with hcp structure, the disappearances of deformation twins have been observed after the subsequent loading processes. For titanium, twins with negative Schmid factors are tend to de-twinning so as to accord with the macroscopic strain [7]. Similarly, for magnesium and its alloys, twins generated under compressive stress would de-twin in subsequent tensile stress.

Furthermore, the cyclic tension and compression tests will lead to the repeated twinning/de-twinning processes [8,9]. For beryllium, constitutive models incorporating the de-twinning process during strain path change are able to predict well the mechanical response and the microstructure evolution [10,11]. Since  $\alpha$ -U can be considered as distorted hcp structure with the  $b$  direction being elongated [12], it is necessary to analyze whether a similar twinning/de-twinning process occurs in  $\alpha$ -U.

Deformation twins induced by external loading are also a complex issue in  $\alpha$ -U because of its double lattice structure and anisotropic mechanical response [13–15]. Crocker et al. [16] predicted theoretically that  $\alpha$ -U has 41 kinds of possible twinning modes based on the principle of minimum twinning shear and atomic shuffle. However, the operative twin modes relate to not only the intrinsic properties of material, such as crystal orientation [17,18] and grain size [19–22], but also the external conditions, such as temperature [17,23–26], pressure [27], strain rate [28–31] and etc.

Recently, Ardeljan et al. [32] reported a model within an explicit finite element framework to calculate the stress fields upon twin formation and propagation in cast uranium. Their simulation is able to relate spatially resolved field of stress and strain with evolution of deformation twin. Knezevic et al. [33,34] integrated the

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viscoplastic self-consistent (VPSC) polycrystalline model with dislocation density within an implicit finite element framework to simulate the macro-scale mechanical response and the micro-scale multiple slip and twinning modes of  $\alpha$ -U. The model captures accurately the tension-compression asymmetry of  $\alpha$ -U associated with twinning.

To date, twin types that have been observed experimentally are summarized in Table 1. Among these twins,  $\{130\}\langle 3-10\rangle$  is the most frequently observed twin mode and  $\{210\}\langle 1-20\rangle$  is a newly found twin type observed by McCabe et al. [35] using electron backscattered diffraction (EBSD) technique. As Table 1 shows, twinning behavior in  $\alpha$ -U is very plentiful, and new twinning behaviors might be observed with advances in twin analysis techniques.

Recent advances in EBSD and focused ion beam (FIB) combined transmission electron microscopy (TEM) techniques greatly promote the microstructure analysis in  $\alpha$ -U, including determination of cleavage fracture surface [20,35], re-crystallization [36,37] and texture analysis [38].

In this study, twinning behaviors of a focused grain and its neighbor grains in  $\alpha$ -U subjected to different compressive strains were investigated using EBSD. In addition, the TEM combined with FIB was used to identify the type of twinning in specific region. Two new deformation microstructures were observed. (1) Some  $\{130\}$  twins in cast uranium disappeared during subsequent compression deformation, which can be interpreted by the Schmid law; (2) Twin pairs of  $\langle -176\rangle$ – $\langle -17-2\rangle$  generated in the adjacent grains were observed. The misorientation and geometric matching between the twin pairs were discussed.

## 2. Materials and methods

The starting material was cast uranium with initial size of  $10 \times 6.6 \times 4.5 \text{ mm}^3$ . Three indentations made by hardness tester on the original surface were taken as the markers to locate the interesting grains.

Compression tests were performed on an electronic universal material testing machine in a nominal strain rate of  $2 \times 10^{-4} \text{ s}^{-1}$  with the displacement control mode. Sample was strained to 4.2% and 6.2%, respectively. Before and after each compression, the sample was transferred into scanning electron microscopy (SEM) chamber for EBSD measurements. As EBSD patterns can be hardly detected after the second deformation due to the severely distorted surface, we re-prepared the sample surface to locate the interesting grain in terms of the markers.

Sample for EBSD measurement was prepared using a two-step electropolish process [36]. EBSD scans were performed at 25 kV with scan step size  $0.3 \mu\text{m}$  in a Sirion 200 SEM equipped with an EDAX/TEAM data acquisition system. The orientation data was analyzed using EDAX/TSL OIM Analysis 7 software. The

compression direction (CD), width direction (WD) and normal direction (ND) of sample were defined as the  $[010]$ ,  $[100]$  and  $[001]$  axes of the sample reference frame during EBSD measurements, as is shown in Fig. 1. Foil for TEM was prepared using an FIB instrument.

To calculate the Schmid factors (SFs) of twins, we firstly transformed the  $[010]$  index from the sample reference frame into the twin reference frame by means of coordinate transformation. Then the angle  $\theta$  between CD and the twinning plane normal, and the angle  $\eta$  between CD and the twinning direction could be obtained. So the Schmid factor  $\mu$  could be calculated in terms of the relation  $\mu = \cos\theta \cdot \cos\eta$ .

The geometric compatibility factor  $m'$  proposed by Luster and Morris [42] was adopted to analyze the geometric matching of twin pairs formed in the adjacent grains. Here  $m' = \cos\kappa \cdot \cos\psi$ ,  $\kappa$  is the angle between two twinning direction of the twin pairs,  $\psi$  is the angle between two twinning plane normals of the twin pairs. The geometric compatibility factor  $m'$  ranges from 0 to 1. If the twin pairs are well matched, the  $m'$  value is close to 1. Conversely, the  $m'$  value is close to 0. To obtain the angle values of  $\kappa$  and  $\psi$ , the indices of twinning plane normal and twinning direction in the twin coordinate system of one side were transformed into the twin coordinate system of the other side.

## 3. Results and discussion

### 3.1. SEM morphology under different strains

Fig. 2 shows SEM images of the area of interest on the uranium surface under different strains. The surface prior to deformation is shown in Fig. 2(a), where three indentations are clearly seen on the right side of the focused grain A within red circle. The black arrow denotes compressive direction. The surface strained to 4.2% is shown in Fig. 2(b), in which the upper and lower circled areas are magnified in Fig. 2(d) and (e), respectively. As Fig. 2(d) shows, the white bands with lens shape and width about  $4 \mu\text{m}$  are  $\langle -130\rangle$

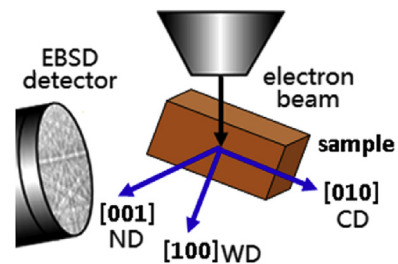


Fig. 1. Illustration of sample reference frame during EBSD measurement. The compression direction (CD), width direction (WD) and normal direction (ND) of sample were defined as the  $[010]$ ,  $[100]$  and  $[001]$  axes, respectively.

Table 1  
Experimentally observed twin types in  $\alpha$ -U.

No.	$K_1$	$K_2$	$\eta_1$	$\eta_2$	Shear	Type	Sources
1	$\{130\}$	$\{1-10\}$	$\langle 3-10\rangle$	$\langle 110\rangle$	0.299	Compound	[1,23,39–41]
2	$\{110\}$	$\{1-30\}$	$\langle 1-10\rangle$	$\langle 310\rangle$	0.299	Compound	[30]
3	$\{112\}$	$\{1-72\}$	$\langle 3-72\rangle$	$\langle 312\rangle$	0.228	I	[1,16,23,39–41]
4	$\{1-72\}$	$\{112\}$	$\langle 312\rangle$	$\langle 3-72\rangle$	0.228	II	[1,23,39–41]
5	$\{111\}$	$\{17-6\}$	$\langle 15-6\rangle$	$\langle 512\rangle$	0.214	I	[16]
6	$\{17-6\}$	$\{111\}$	$\langle 512\rangle$	$\langle 15-6\rangle$	0.214	II	[23,39]
7	$\{021\}$	$\{1-114\}$	$\langle -26-12\rangle$	$\langle 132\rangle$	0.286	I	[16]
8	$\{121\}$	$\{1-41\}$	$\langle 3-21\rangle$	$\langle 311\rangle$	0.329	I	[1,23,39–41]
9	$\{210\}$	–	$\langle 1-20\rangle$	–	–	I	[35]

Note: Apostrophes represent the irrational indices.

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