

Simulation of Texture Evolution during Uniaxial Deformation of Commercially Pure Titanium

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Abstract: The evolution of texture in commercially pure (CP) titanium during uniaxial tension and compression through VPSC (Visco-plastic self-consistent) simulation is reported in the present study. CP-titanium was subjected to both uniaxial tension and compression upto 35% deformation. During uniaxial tension, tensile twin of $\{10\bar{1}2\}<\bar{1}011>$ type and compressive twin of $\{11\bar{2}2\}<11\bar{2}3>$ type were observed in the samples. However, only tensile twin of $\{10\bar{1}2\}<\bar{1}011>$ type was observed in the samples during uniaxial compression. Volume fractions of the twins were increased linearly as a function of percentage deformation during uniaxial tension. Whereas, during uniaxial compression the twinning volume fraction was increased up to 20% deformation and then decreased rapidly on further increasing the percentage deformation. During uniaxial tension, the general t-type textures were observed in the samples irrespective of the percentage deformation. The initial non-basal texture was oriented to split basal texture during uniaxial compression of the sample. VPSC formulation was used for simulating the texture development in the material. Different hardening parameters were estimated through correlating the simulated stress-strain curve with the experimental stress-strain data. It was observed that, prismatic slip $\{10\bar{1}0\}<11\bar{2}0>$ operated as the primary deformation mode during uniaxial tension whereas basal slip $\{0001\}<11\bar{2}0>$ acquired the leading role during deformation through uniaxial compression. It was also revealed that active deformation modes were fully depending on percentage deformation, loading direction, and orientation of grains.

Keywords: Tension, Compression, Texture, EBSD, XRD, VPSC

1. Introduction

Titanium and its alloys are most widely used for structural, chemical, automobiles, and medical application due to its large specific strength and excellent corrosion resistance [1-3]. Evolution of texture and microstructure in hexagonal material, thus, needs to be further exploited. Further VPSC simulation is successfully used to understand the texture developments in cubic as well as hexagonal materials [4-7]. In polycrystalline materials, the imposed plastic strain is accommodated by various active deformation mechanisms such as dislocation movement in a confined circumstance. Both slip and twin are the important deformation modes for dislocation movement in hcp material such as titanium [8, 9]. The activation of slip systems is generally depending upon the shear stress between two gliding planes, and angle between crystals and loading directions. In titanium, the most favorable slip systems being the prismatic slip with a-type Burgers vectors followed by basal and pyramidal slips with a-type Burgers vectors [10]. However according to Von Mises's, five independent slip systems are required for arbitrary shape change during the plastic deformation of polycrystalline titanium [11]. So pyramidal $\langle a+c \rangle$ slip or deformation twinning has to be activated during deformation in plastic range of hexagonal titanium [12]. The activities of slip and twin systems at room temperature deformation of pure titanium are observed to be mostly in the order of prismatic slip, basal slip, tensile twin, compressive twin and 1st order pyramidal slip



[13]. So pyramidal $\langle a+c \rangle$ slip or deformation twinning has to be activated during plastic deformation of hexagonal titanium [14].

Various authors have been exploited the texture evolution through different strain-paths. A dominant basal texture has been observed during uniaxial tension and compression of cp-titanium at room temperature [15, 16]. However, evolution of texture and microstructure during tensile and compression deformation along with modeling of texture has not been reported elsewhere. With this background study, in the present study the evolution of texture during tensile and compression deformation of cp-titanium has been investigated through experimentation and simulation.

2. Experimental details

(a) Material

CP-titanium (Grade-2) of 1mm thick sheet and 10mm diameter rod were used for uniaxial tension and compression respectively. The chemical composition (in wt %) of the material is shown in Table 1. Both tensile and compression specimens (Figure 1.) were prepared by using wire EDM (Electrical Discharge Machining) technique.

Table 1. Chemical composition of the material

Ti	Fe	C	N	H	O
0.820	0.034	0.004	0.004	0.004	0.134

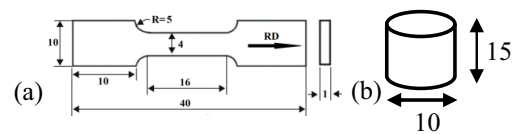


Figure 1. Schematics of (a) tensile and (b) compression specimen used (all are in mm)

(b) Uniaxial Tension

Tensile deformation was carried out along rolling direction of the specimen in an Instron 5567 screw driven UTM (universal testing machine) at room temperature. Subsequently, different specimens were subjected to tensile deformations of 5, 15, 25, and 35% deformation at the strain rate of $1 \times 10^{-3} \text{ s}^{-1}$.

(c) Uniaxial Compression

Compression deformation was carried out similar to the extrusion direction (ED) of the specimen in an Instron 5567 screw driven UTM (universal testing machine) at room temperature. Different specimens were subjected to compression of 3, 10, 20, and 30% deformation at the strain rate of $1 \times 10^{-3} \text{ s}^{-1}$.

(d) Sample Preparation

Deformed region of the samples were polished metallographically followed by electro-polished prior to the textural and microstructural characterizations. Metallographic polishing was accomplished in a Struers Labopol using different grit of SiC grinding papers, while electro-polishing was accomplished in a Struers Lectropol-5 using an electrolyte of methanol and perchloric acid (80:20) at -20°C and 25V for 12sec.

(e) X-Ray Diffraction (XRD)

A Bruker D8 Advance XRD setup with Co $K\alpha$ radiation was used to measure the bulk texture of the samples. (0002) pole figure was measured and was calculated using Labotex V 3.0 software.

(f) Electron Backscattered Diffraction (EBSD)

For the EBSD measurement of the samples, a FEI Quanta-3D-FEG scanning electron microscope was used. An approximately $1 \text{ mm} \times 1 \text{ mm}$ area from two different locations of the samples was scanned using a step size of $0.5 \mu \text{m}$. Both video and beam conditions were kept constant between the scans. A TSL-OIM Version 6.2 EBSD package was used for the analysis of the EBSD scans.

3. VPSC (Viscoplastic Self Consistent) Simulation

To pursue the effect of deformation on texture evolution during the deformation of cp-titanium in plastic range, visco-plastic self-consistent simulation was accomplished using the VPSC-7 software package. Deformation of the material was based on the mechanisms of crystal plasticity, where systems of slip and twin were activated by their respective resolved shear stress. The response of the single crystal is expressed with the help of rate sensitive constitutive law.

$$\dot{\epsilon}_{ij}(\bar{X}) = \sum_s m_{ij}^s \dot{\gamma}^s(\bar{X}) = \dot{\gamma}_0 \sum_s m_{ij}^s \left(\frac{m_{kl}^s \sigma_{kl}(\bar{X})}{\tau_0^s} \right)^n \quad (1)$$

Where ' $\dot{\epsilon}$ ' denotes strain rate in the grain, ' m^s ' denotes the geometric of Schmid tensor, ' s ' denotes a label for slip systems, ' τ^s ' denotes threshold stress to control the activation of a slip system and ' n ' implies the rate sensitivity. The activation of slip system leads to self or latent hardening of it due to the activation of same slip system or any other slip system respectively. This is outlined by an empirical Voce law given as:

$$\hat{\tau}^s = \tau_0^s + (\tau_1^s + \theta_1^s \gamma)(1 - \exp(-\gamma \frac{\theta_0^s}{\tau_1^s})) \quad (2)$$

Where $\gamma = \sum_s \Delta \gamma^s$ is the accumulated shear in the grain; $\tau_0, \theta_0, \theta_1, (\tau_0 + \tau_1)$ are the initial CRSS value, the initial hardening rate, the asymptotic hardening rate and the back-extrapolated CRSS value respectively. While θ_0 and τ_1 are typically positive, their absolute values are used in (2) in order to entertain few special cases.

In this investigation, VPSC code with the intermediate $n^{\text{eff}} = 10$ approach was taken for modelling the deformation texture. The effect of strain path was modelled using a process IVGAR=0; where the code will impose the same velocity gradient in each step. In order to simulate the texture development during tensile and compression deformation, nearly 4000 random orientations were taken. The simulation was carried out till $\varepsilon = 0.35$ for tensile deformation using velocity gradient $L_{11} = 1, L_{22} = -0.5, L_{33} = -0.5$ and $L_{12} = L_{13} = L_{21} = L_{23} = L_{31} = L_{32} = 0$ and till $\varepsilon = 0.3$ for compression deformation using velocity gradient $L_{11} = 0.5, L_{22} = 0.5, L_{33} = -1$ and $L_{12} = L_{13} = L_{21} = L_{23} = L_{31} = L_{32} = 0$. Five deformation modes such as prismatic slip $\{10\bar{1}0\} \langle 11\bar{2}0 \rangle$, basal slip $\{0001\} \langle 11\bar{2}0 \rangle$, pyramidal slip $\{10\bar{1}1\} \langle 11\bar{2}3 \rangle$, tensile twin $\{10\bar{1}2\} \langle \bar{1}011 \rangle$ and compression twin $\{11\bar{2}2\} \langle 11\bar{2}3 \rangle$ were activated to match the stress strain curve obtained by simulation with experimental curve. The values of the hardening parameters for the best fit of the deformation through compression and tension are shown in table.2.

Table 2. Hardening parameter of deformation modes used for the simulation

Slip/Twin	τ_0	τ_1	θ_0	θ_1
Prismatic	110	20	600	120
Basal	170	60	1200	90
Pyramidal<a+c>	220	100	600	75
Tensile twin	120	120	500	150
Compression twin	180	110	1000	250

4. Results

4.1 Evolution of Microstructure and Texture

4.1.1 Uniaxial Tension

The microstructures (map) of the deformed samples as a function of % deformation are shown in **Figure 2**. The starting material had an equiaxed grain structure of average grain size of $\sim 75 \mu\text{m}$. Both $85^\circ \langle 11\bar{2}0 \rangle$ type of tensile twins (red in colour) and $64.3^\circ \langle 1100 \rangle$ type of compression twins (blue in colour) were significantly observed during the deformation of the samples.

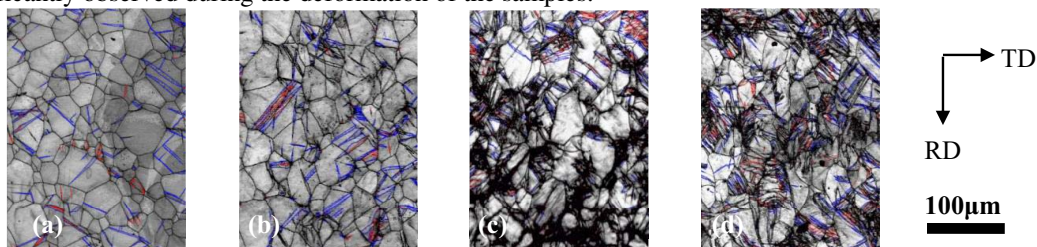


Figure 2. Microstructure maps (IQ) of deformed cp-titanium subjected to tensile loading of (a) 5%, (b) 15%, (c) 25%, and (d) 35% deformation

In **Figure 3(a)**, the twin boundary length in the deformed materials is shown as a function of percentage deformation of the samples. It was observed that, twin boundary increased with increasing the % deformation. However the rate of activation of tensile twin was more with respect to compression twin. The average grain size as a function of % deformation during tensile deformation is shown in **Figure 3(b)**. A progressive decrease in grain size with increasing % deformation was observed. The misorientation angle development within the grain of the deformed material during deformation is shown in **Figure 3(c)**. It represents the average misorientation angle was increased with progressive deformation of the samples.

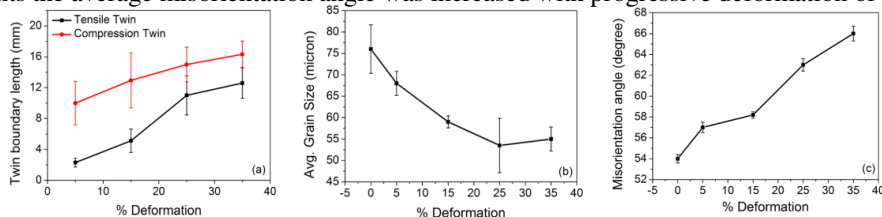
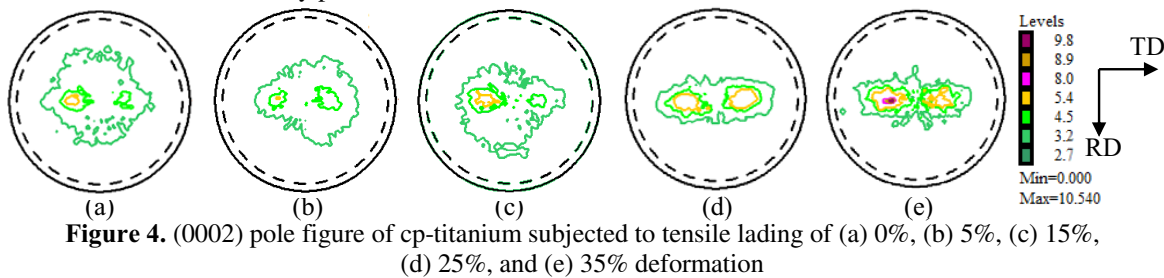


Figure 3. Distribution of (a) Twin boundary length, (b) average grain size and (c) misorientation angle w.r.t % deformation during tensile loading of cp-titanium

The texture evolutions in the deformed specimen of cp-titanium were represented by (0002) pole figure as shown in **Figure 4**. The initial sample had typical t-type texture, which also known as split basal texture inclined at 35° away from normal direction (ND) towards transverse direction (TD). The texture got strengthened with progressive deformation however position of maximum level of intensity of split basal texture remained at the early position.



4.1.2 Uniaxial Compression

Figure 5 represents the microstructure of deformed samples during compression in the form of map. Un-deformed material with most of the grains oriented in the non-basal orientation had an equiaxed grain of $\sim 14\mu\text{m}$ average size. It was observed that grain with non-basal orientations were prone to twinning. $85^\circ \langle \bar{1}2\bar{1}0 \rangle$ type of tensile twin (red in color) was observed in significant quantity up to 20% deformation and then decreased as shown in **Figure 6(a)**. Average grain sizes, and misorientation angle development of deformed material with respect to percentage deformation during compression were shown in **Figure 6(b)** and **Figure 6(c)** respectively. It was observed that, average grain size of the grain decreased linearly with increase in deformation percentages. The misorientation development inside the specimen during deformation was increased up to 20% deformation and then decreased on further deformation.

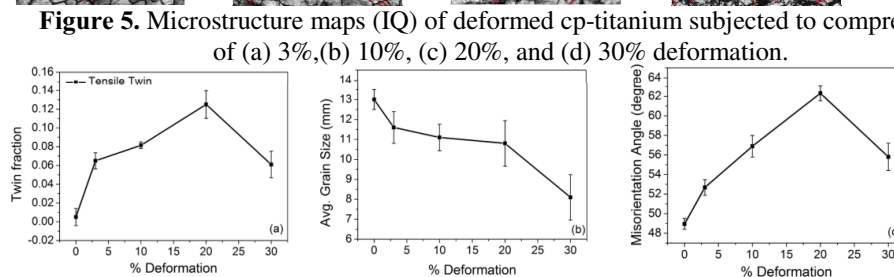
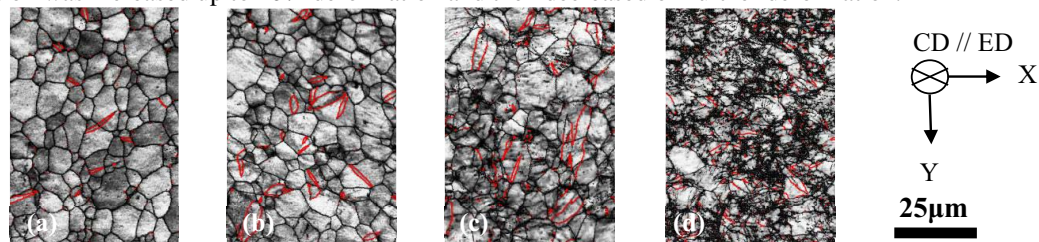
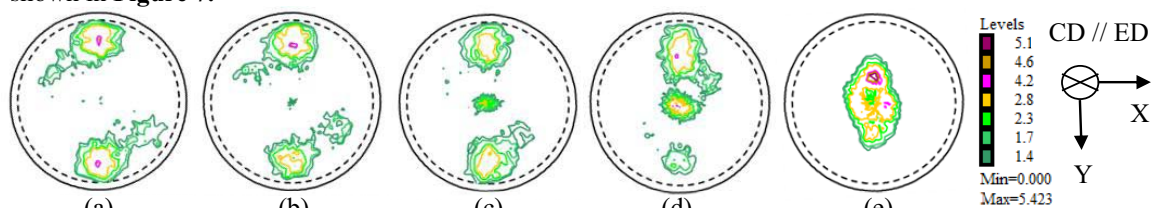


Figure 6. Distribution of (a) Twin boundary fraction, (b) average grain size and (c) misorientation angle w.r.t % deformation during compressive loading of cp-titanium

The texture evolution in deformed material during compression was represented by (0002) pole figure as shown in **Figure 7**.



The initial non basal texture of the un-deformed material was oriented towards basal texture during the compression. On further deformation, it ended with split basal texture.

4.2. VPSC Simulation

Hardening parameters (Table 2) were obtained from the best fit experiment and simulated true stress-strain curve of both tensile and compression Figure 8(a) & 9(a). The activity curve for the various deformation modes were plotted as shown in Figure 8(b) & 9(b). The (0002) pole figures of the deformed material obtained by simulation were shown in Figure 10 & 11. A considerable match is observed between simulated and experimental (0002) pole figure of both tensile and compression deformed material.

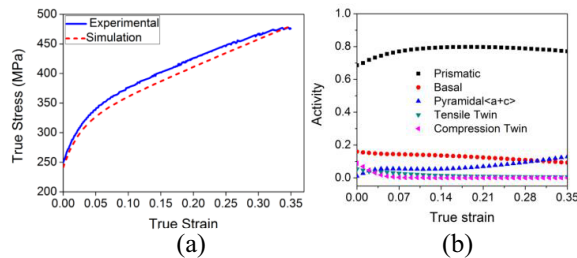


Figure 8. (a) Comparison between experimental and simulated true stress-strain curve, (b) Activity of various deformation modes of cp-titanium material subjected to 35% deformation

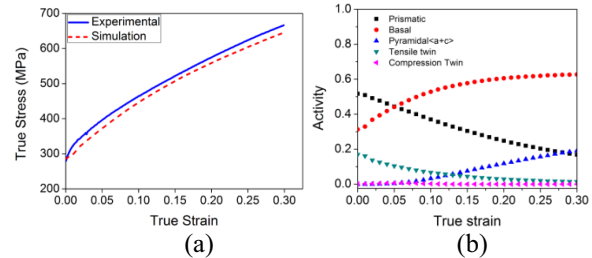


Figure 9. (a) Comparison between experimental and simulated true stress-strain curve, (b) Activity of various deformation modes of cp-titanium material subjected to 30% compression loading

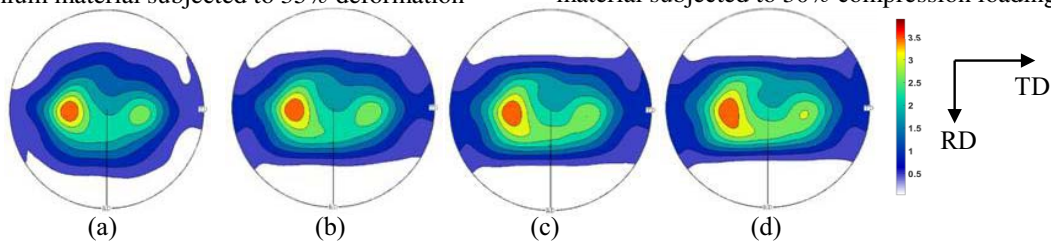


Figure 10. Simulated (0002) pole figure of cp-titanium at (a) 5%, (b) 15%, (c) 25%, and (d) 35% deformation during tensile loading

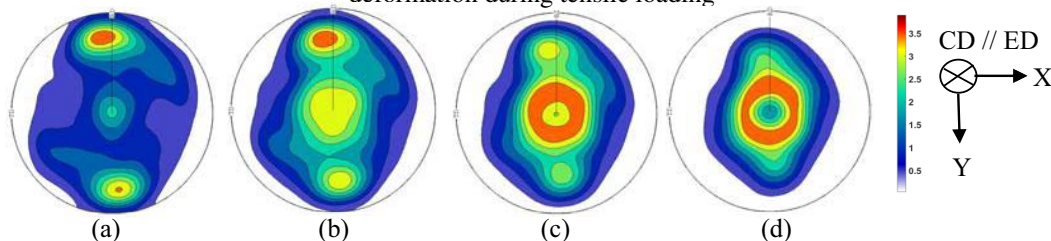


Figure 11. Simulated (0002) pole figure of cp-titanium at (a) 3%, (b) 10%, (c) 20%, and (d) 30% deformation during compressive loading

In tensile deformation, prismatic slip system was activated as primary deformation mode and its contribution to overall deformation was higher. However the contributions of both twins were significant at the low strain for accommodating strain and diminished at higher strain. The slip activity obtained from the simulation indicated that, higher number of deformation modes was activated throughout the compression as compared to the tensile deformation. In compression, basal slip acted as preliminary deformation mode. At lower strain both prismatic slip and tensile twin played important role for plastic deformation. However at the high strain, basal and pyramidal slip systems were activated for accommodating the imposed strain.

5. Discussion

The difference in texture and microstructure during the deformation of both tensile and compression material was observed from both bulk and EBSD texture data. In tensile deformation, grains were fragmented due to the initial contribution of both tensile and compression twin. Grains with high schmid factor were prone to twinning during the deformation. With increase in further deformation, the average misorientation angle was increased due to the continuous presence of the twin boundary which comprises

both 85° and 64° misorientation in between the two adjacent boundary. Similarly the texture development was remained more or less same throughout the deformation of cp-titanium. This is due to the less participation of twin during the deformation and their sharing towards the evolution of preferred orientation was very less as compared to parent grain. From the VPSC, it has been anticipated that most of the grains in the material oriented along their prismatic slip plane along $\langle 11\bar{2}0 \rangle$ direction, and leads to forming split basal texture throughout the deformation. One can conclude that extension and contraction twinning were responsible for the grain refinement only and not for the texture evolution during the tensile deformation of cp-titanium material.

During compression deformation, the evolution of texture and microstructure were observed due to the presence of tensile twin of 85° type $\langle 12\bar{1}0 \rangle$. The average grain size of the deformed grain was decreased with increase in deformation percentage due to the activation of tensile twin. Non basal grains with high Taylor factor value were prone to twinning. The fraction of twin increased with deformation percentage up to 20% and then decreased this may be due to the twin inhalation of whole grain during the deformation. At the higher deformation, all twin boundaries were converted to normal grain boundary with lesser misorientation in between twin grain and neighbour grain. So decrease in twin volume fraction and average misorientation angle was observed at the high deformed material. Similarly average misorientation angle increased up to 20% and then decreased for the above explained reason. The said tensile twin was also responsible for the 85° rotation of the non-basal oriented grain into basal direction in the initial stage of compression. On further increasing the deformation percentage, contribution of basal slip was more and played a role for the formation of split basal texture.

6. Conclusion

From VPSC simulation, it has been observed that prismatic slip acts as primary deformation mode during the tensile deformation. Both the twins have larger contribution towards accommodating imposed strain in the low strain deformation however their contribution is low at higher strain. In compression deformation, both microstructural and textural evolution has taken place due to the dominant tensile twin. Similarly basal slip acts as preliminary deformation mode for the deformation. It can be concluded that microstructure and texture evolution during the deformation of the cp-titanium material is dependent on the initial orientation of grain, direction of loading and size of the grain.

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