Article

Constitutive Analysis of the Anisotropic Flow Behavior of Commercially Pure Titanium

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Received: 23 October 2020; Accepted: 9 November 2020; Published: 10 November 2020

Abstract: Plastic anisotropy is an important issue for metals possessing a hexagonal close-packed structure. This study investigated the anisotropic deformation characteristics of commercially pure titanium with basal texture. A quasi-static uniaxial compression gave rise to clear differences in flow curves and strain-hardening rates depending on the loading direction. This study employed a constitutive approach to quantify the contribution of (i) dynamic Hall–Petch strengthening, (ii) dislocation pile-up, and (iii) texture hardening with respect to the total flow stress. Such an approach calculated a flow stress comparable to the measured value, providing logical validity. The microstructural and mechanical differences depending on the loading direction (i.e., anisotropy) were successfully interpreted based on this approach.

Keywords: titanium; plastic anisotropy; flow curve; constitutive analysis

1. Introduction

Titanium and its alloys are used in many commercial applications in the aerospace, biomedical, sporting goods, and sea water plant industries [1–3]. Such a wide application is attributed to the high specific strength, biocompatibility, and high corrosive resistance of these alloys. Among various alloy variants, commercially pure titanium (CP-Ti) has been used in the applications of heat exchangers or pressure vessels due to its remarkable corrosive resistance and cold formability. It also has an economical benefit from excluding expensive alloying elements such as Nb, Ta, and Hf [4].

Besides its engineering advantages, CP-Ti possesses a significant anisotropy of mechanical behaviors due to the intrinsic nature of its hexagonal close-packed structure [5]. In other words, the plastic deformation behavior of CP-Ti considerably varies depending on the direction of the applied loading. A conventional rolling process gives rise to a strong split basal texture in CP-Ti, where (i) {0002} basal planes are aligned with the rolling direction (RD) and (ii) the basal axis is tilted from the normal direction (ND) to the transverse direction (TD) in the cross-section [6]. Such a preferential texture development resulted in plastic anisotropy, as mentioned above.

An effective way to interpret the mechanical and/or microstructural behaviors of CP-Ti, including plastic anisotropy, is a constitutive analysis. Such an approach establishes a constitutive equation correlating various physical quantities, providing an estimation of the specific properties under a given condition. For example, Lee et al. [7] made a highly accurate prediction for the transient stress drop of electropulsing-treated CP-Ti utilizing the modified Johnson–Cook model integrated with the term of dynamic strain aging. Asim et al. [8] employed a representative volume element simulation to model a void formation at the phase interface of titanium alloys. Siddiq et al. [9,10] modified a full-variation porous plasticity model to interpret the void coalescence of ductile metals.

This study aims to clarify the role of anisotropy in microstructural evolution and the compressive deformation properties of rolled CP-Ti sheets. The plastic deformation behaviors were investigated depending on the loading direction of RD, ND, and TD. In addition, our research novelty is the introduction of a constitutive approach to divide flow stress into three stress components representing a dynamic grain refinement, dislocation pile-up, and texture hardening. Such an approach assists in measuring the contribution of each stress component to the total plastic deformation behavior depending on the loading direction. Furthermore, this approach requires a significantly lower number of parameters as compared with the microstructure-based numerical models in the literature [8–10].

2. Materials and Methods

Grade 2 CP-Ti plate was investigated in this study. The plate was hot-rolled at 973 K up to a thickness of 10 mm, which corresponded to an area reduction of 75%. It was then subsequently annealed at 933 K for 1 h to decrease the dislocation density and to promote a sufficient grain growth for the activation of mechanical twinning. Quasi-static uniaxial compression tests (8801, INSTRON, Norwood, MA, USA) were conducted at a strain rate of 10^{-2} s^{-1} in an ambient atmosphere. For this purpose, cylindrical specimens were machined along one of three directions (i.e., RD, ND, and TD) with a 7 mm in diameter and 7 mm length (Figure 1). The compression tests were repeated three times for each condition for the following experiments as well as the data reproducibility. After the test, two of three specimens were soaked in a furnace (AWF13, Lenton, Hope Valley, UK) at 773 K for 12 h to remove piled-up dislocations and then compressed again to evaluate the change in yield strength (YS). The final specimens, after the compression test, were used for microstructural and textural characterizations using the electron backscatter diffraction (EBSD, FEI QUANTA 3D FEG, Hillsboro, OR, USA) technique. The samples were mechanically polished with #400, #800, #1200, and #2400 SiC paper. They were then subjected to electropolishing equipment (LectroPol-5, STRUERS, Denmark) at 22 V for 30 s in a solution of 410 mL methanol, 2450 mL ethylene glycol butyl ether, and 40 mL perchloric acid. The EBSD data were obtained at a step size of $1.3 \mu\text{m}$ and then processed using the TSL OIM ver. 7 software (EDAX, Mahwah, NJ, USA). Low-confidence-index (<0.1) data were excluded for this processing to secure data reliability.

Figure 1. Schematic illustration of cylindrical specimens for quasi-static uniaxial compression test. They were machined along rolling direction (RD), normal direction (ND), and transverse direction (TD), respectively.

3. Results

The initial microstructure of the rolled CP-Ti sheet was investigated through EBSD analysis (Figure 2). The inverse pole figure map showed an equiaxed grain structure with an average grain size of $55 \mu\text{m}$. In addition, the split basal texture was confirmed in the initial microstructure; most basal poles were tilted by approximately $20\text{--}40^\circ$ from ND towards TD, while maintaining the perpendicularity to RD. This is the typical characteristic of rolled CP-Ti sheet, as reported earlier [6].

Figure 2. EBSD (electron backscatter diffraction) investigation for the initial microstructure: (a) inverse pole figure map from the 3-dimensional view and (b) pole figures with respect to (0001), (11–20), and (10–10).

The uniaxial compression along RD, ND, and TD gave rise to two obvious differences in the flow behavior of CP-Ti (Figure 3). First, the alloys exhibited different YS values depending on the compressive direction: 144 MPa for RD, 202 MPa for ND, and 182 MPa for TD. Such an anisotropic behavior originated from the difference in the critical resolved shear stress (CRSS) and the Schmid factor (SF) for favorable slip systems [11]. This is further discussed in the following paragraph with the calculated SF values for the present case. The flow stresses measured at a compressive strain of 0.2 were comparable in spite of the lowest YS for the RD specimen. Second, an anisotropic strain-hardening behavior was revealed in Figure 3b. RD and ND compressions resulted in the three-stage hardening [12]; the hardening rate decreased in Stage A, increased due to the activation of twinning in Stage B, and then decreased again after the twinning saturation in Stage C. The specimen compressed along ND, however, showed significantly less increase in hardening rate in Stage B compared to the RD specimen. Meanwhile, the TD compression led to a monotonic reduction in the strain-hardening rate. The comparable flow curves after a compressive strain of 0.2, as shown in Figure 3a, stemmed from the highest strain-hardening rate of RD.

Figure 3. Compressive deformation behavior of CP-Ti (commercially pure titanium) depending on the loading direction: (a) flow stress curves starting from the yield point and (b) strain-hardening rates.

SF values (m) determine the quantitative relation between the applied normal stress (σ) and resolved shear stress on a given slip plane (τ), expressed as follows [11]:

$$\tau = m\sigma = \cos(\phi)\cos(\lambda)\sigma, \quad (1)$$

where ϕ and λ are an angle of the axial force vector and shear force vector, respectively, with respect to the normal vector of the given plane. Slip is initiated when the resolved shear stress exceeds CRSS for each slip plane. Accordingly, a high SF value makes slip liable to occur, thereby decreasing YS. The SF values for each compressive direction were calculated for prismatic $\langle a \rangle$ slip (Figure 4), because it is the most favorable slip system in CP-Ti with the rolling texture at room temperature [13]. In the initial state (i.e., before the compression), RD presented the highest SF value on average, thereby rationalizing its lowest YS, as shown in Figure 3a. Similarly, the highest YS of the ND specimen is understood in light of the lowest SF value on average. Such results are further supported by consistent conclusions made in a previous work [13] that the basal slip is the most favorable slip system in ND compression.

Figure 4. Distribution of the SF (Schmid factor) values for prismatic slip before and after applying a compressive strain of 0.2: (a) RD, (b) ND, and (c) TD.

EBSD analysis suggested the types and fractions of twinning for the compressed CP-Ti alloys (Figure 5). Twin boundaries were detected on the basis of a tolerance misorientation of 5° . $\{10\text{--}12\}$ extension twinning and $\{11\text{--}22\}$ compressive twinning were dominant in compression along the RD and ND, respectively, while both twinning systems were competitive in compression along TD. In detail, the area fraction of the $\{10\text{--}12\}$ twins was 45.1% for RD, 8.1% for ND, and 8.3% for TD. The fraction of $\{11\text{--}22\}$ was 11.1%, 39.2%, and 11.3%, respectively. Interestingly, the RD and ND compressions exhibited different behavior for the hardening rate, as shown in Figure 3b, despite their similar twin fractions. The negligible increase in the strain-hardening rate shown in the ND specimen arose from the difference in the activated twinning system. This is further discussed in Section 4 based on a constitutive analysis.

Figure 5. EBSD image quality map with marked twin boundaries at a compressive strain of 0.2 along (a) RD, (b) ND, and (c) TD. Red and blue lines indicate {10–12} and {11–22} twin boundaries, respectively.

4. Discussion

A constitutive approach was employed to quantify the contribution of microstructural factors to the plastic deformation behavior in order to provide deeper insight into the CP-Ti anisotropy. The flow stress at a compressive strain of 0.2 ($\sigma_{0.2}$) is composed of the stress component related to the dynamic Hall–Petch strengthening ($\Delta\sigma_{H-P}$), dislocation pile-up ($\Delta\sigma_{disl}$), and texture hardening ($\Delta\sigma_{tx}$), as well as YS (σ_y), expressed as:

$$\sigma_{0.2} = \sigma_y + \Delta\sigma_{H-P} + \Delta\sigma_{disl} + \Delta\sigma_{tx}. \quad (2)$$

The dynamic Hall–Petch strengthening is determined by the reduction in the effective grain size, as follows:

$$\Delta\sigma_{H-P} = k_y(d_f^{-0.5} - d_i^{-0.5}), \quad (3)$$

where k_y ($= 0.53 \text{ MN}\cdot\text{m}^{-1.5}$, [14]) is a material coefficient, d_i is the initial grain size, and d_f is the effective grain size determined by high-angle boundaries with a misorientation angle higher than 15° . The active occurrence of mechanical twinning stimulates a significant grain refinement and resultant dynamic Hall–Petch strengthening. Regarding the investigated loading directions, RD compression gave rise to the highest $\Delta\sigma_{H-P}$ value (83 MPa), followed by ND compression (69 MPa) and TD compression (30 MPa). The markedly low $\Delta\sigma_{H-P}$ value of the TD specimen is rationalized by the suppressed twinning.

For further analysis, the 20%-compressed specimens were subsequently annealed at 773 K for 12 h; this condition was set to induce the recovery while suppressing the static recrystallization as much as possible. In other words, the dislocations generated by the compression were annihilated without changing granular and textural structures. Such a heat treatment enabled us to investigate the influence of dislocation hardening (i.e., $\Delta\sigma_{disl}$ values) by excluding the other stress components. The measured $\Delta\sigma_{disl}$ values demonstrate a clear tendency. RD and ND compression made comparable values (69 MPa and 74 MPa), whereas TD compression showed a remarkably larger dislocation hardening (114 MPa).

Finally, the texture hardening of each sample was evaluated from the strain accommodated by mechanical twinning (ε_{tw}) at a compressive strain of 0.2, as follows [14]:

$$\varepsilon_{tw} = sf_{tw}/\sqrt{2}, \quad (4)$$

where s is twin shear (0.217 for {10–12} and 0.176 for {11–22}, [14]) and f_{tw} is the area fraction of mechanical twins. RD and ND specimens exhibited higher ε_{tw} values due to their higher fraction of twinned regions in comparison to the TD sample. It is thus inferred that slip was the primary deformation mechanism in the latter, providing a good explanation for the aforementioned high contribution of dislocation hardening. Meanwhile, the dominant twinning system in the RD compression (i.e., {11–22}) possessed the lower twin shear than the {10–12} twinning system.

This rationalizes the comparable dislocation hardening between the RD and ND specimens in spite of the 10% higher fraction of twinned region in the former.

Activation stress for slip is determined as the ratio of CRSS (τ_{CRSS}) and SF in a single crystal [15]. The activation stress of polycrystalline metal (σ_a) can be calculated by expanding this model as follows:

$$\sigma_a = \Sigma(\tau_{CRSS}/m)n_{SF}, \quad (5)$$

where n_{SF} is the number fraction of SF value. This work calculated the activation stresses for two slip systems (i.e., prismatic and basal slips) in grains with an SF for prismatic slip less than 0.2. The lowest values were selected from these results, providing a CRSS value of 58 MPa for prismatic slip and 95 MPa for basal slip. Either hardening or softening induced by texture development was quantified by the difference between activation stresses before and after applying a compressive strain of 0.2 (i.e., $\sigma_a|_{\epsilon=0.2} - \sigma_a|_{\epsilon=0}$). Consequently, the $\Delta\sigma_{tx}$ values were calculated to be 27 MPa for RD, −10 MPa for ND, and 5 MPa for TD.

Revisiting Figure 4, RD compression gave rise to the most drastic change in SF values after applying a compressive strain of 0.2. The high fraction of lattice orientations favorable for prismatic slip changed into a relatively uniform distribution of SF values due to the activation of {10–12} extension twinning. Such crystal rotation gave rise to an effective texture hardening during RD compression. On the other hand, ND compression induced less change in SF values, even though the ND specimen showed twin characteristics similar to those of the RD specimen. The average SF value for prismatic slip was slightly increased after the deformation, resulting in a weak softening effect. TD compression also caused the small change in SF distribution from moderate to low values, which accompanied weak texture hardening.

The theoretically determined stress components and total stress increment are presented for the investigated compressive directions (Figure 6). The total stress increment was calculated to be 178 MPa for RD, 135 MPa for ND, and 149 MPa for TD. It is of particular note that these data were greatly consistent with the measured stress increments at a compressive strain of 0.2: 180 MPa for RD, 140 MPa for ND, and 151 MPa for TD. This supports the logical validity of the constitutive approach adopted in this work.

Figure 6. Contribution of stress components to the flow stress increment at a compressive strain of 0.2 based on the constitutive analysis.

5. Conclusions

This study adopted the constitutive approach to divide the flow stress of CP-Ti into three stress components representing dynamic grain refinement, dislocation pile-up, and texture hardening. The constitutive analysis adopted by the present study successfully predicted the stress components and provided further insight into the anisotropic deformation behavior of CP-Ti. RD compression induced the highest stress increment due to the most significant decrease in the effective grain size and {10–12} extension twinning accompanying the lattice orientation unfavorable for prismatic slip.

During ND compression, {11–22} compressive twinning gave rise to the lattice orientation favorable for prismatic slip. The specimen also went through the weaker Hall–Petch strengthening. These factors led to the lowest flow stress and a plateau region in Stage B of the strain-hardening rate. TD compression showed the weakest grain refinement due to the suppressed activation of mechanical twinning. However, the primary slip activation resulted in the highest dislocation hardening, which compensated for the low Hall–Petch strengthening.

Author Contributions: Conceptualization, D.K., T.L. and C.S.L.; investigation, D.K. and T.L.; resources, C.S.L.; writing—original draft preparation, D.K. and T.L.; writing—review and editing, T.L. and C.S.L.; supervision, C.S.L. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (Ministry of Science and ICT) (No. 2018R1C1B6002068 & 2020R1A4A3079417).

Conflicts of Interest: The authors declare no known conflict of interest.

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