Technical Report

Deformation Temperature Dependence of Active Twinning Systems during Compressive Deformation in Polycrystalline Commercially Pure Titanium

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Abstract

In order to clarify the effect of deformation temperature on twinning deformation for polycrystalline commercially pure titanium, active twinning systems during compression deformation at temperatures from 25–800°C for JIS Class 1 commercially pure titanium at 0.5 mm in mean grain diameter were investigated using SEM/EBSD techniques. At a reduction of 10%, four twin systems were confirmed to operate depending on the deformation temperature: the $\{11\bar{2}1\}$, $\{11\bar{2}2\}$, and $\{10\bar{1}1\}$ twins were observed at 25–200°C, 25–400°C, and 400–800°C, respectively, while the $\{10\bar{1}2\}$ twins formed at every tested temperature (25–800°C). Those temperature ranges for the $\{10\bar{1}1\}$ twins were the same as those previously reported obtained using single-crystal specimens. However, the others were different between single-crystal and polycrystal specimens, indicating that the effects of stress and/or strain concentration at grain boundaries on twinning are different depending on the twinning systems and deformation temperatures.

1. Introduction

Twinning deformation greatly affects mechanical properties, such as ductility and work hardening properties, and the formation of microstructure (e.g., texture) of commercially pure titanium.[1, 2] Many studies have been performed regarding twinning deformation in commercially pure titanium using single-crystal and polycrystal specimens. It has been reported that as many as four types of twinning systems shown in **Fig. 1** mainly operate depending on the processing procedure and temperature. It has also been reported that active twinning systems, in particular, greatly depend on the processing temperature; for example, in single-crystalline pure titanium, $\{10\bar{1}2\}$ and $\{11\bar{2}2\}$ twins operate at and around room temperature, and $\{10\bar{1}1\}$ twins operate from 400°C to lower than β transformation temperatures.[3] As described above, the temperature dependence of active twinning systems in single crystals has been systematically researched. In polycrystalline materials, in order to maintain the consistency of displacement between adjacent crystal grains near grain boundaries, geometrically necessary (GN) dislocations need to be formed. As a result, GN dislocations accumulate near grain boundaries.[4] For these reasons, it can be considered that many dislocations that have accumulated near grain boundaries of polycrystalline materials cause large stress/strain concentration and thereby twinning deformation behavior of polycrystalline materials differs from that of single crystals. Accordingly, it is very important from an industrial perspective to study twinning deformation behavior in polycrystalline commercially pure titanium and clarify the effect of grain boundaries on each twinning system.

In this study, JIS Class 1 polycrystalline commercially pure titanium materials with coarse crystal grains were compressed at various temperatures and active twinning systems during the compression were studied to clarify the effect of the deformation tempera-

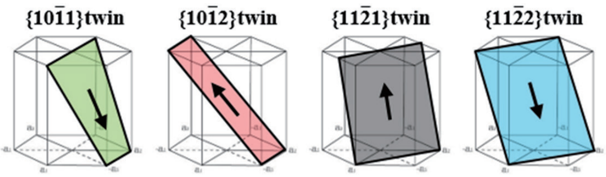

Fig. 1 Twinning systems observed in titanium

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ture on them.

2. Experimental Procedure

As a test sample, JIS Class 1 commercially pure titanium (Ti-0.042O-0.027Fe-0.001N-0.006C-0.0006H, mass% for all) was used. The microstructure of the test sample was equiaxial with a mean crystal grain size of 500 μm, and the texture was almost random. Cylindrical test specimens with a diameter of 8 mm and a height of 12 mm were fabricated from the test sample, and they were subjected to a uniaxial compression test (using a hot-working simulation tester (Thermec-master Z) made by Fuji Electronic Industrial Co., Ltd.). In the uniaxial compression test, the test specimens were heated at various temperatures from 25°C to 800°C. They were retained for 10 minutes at each temperature and compressed by 10% at the strain rate of 1.0 s^{-1}. In addition, to freeze the deformation microstructure, helium gas was used to rapidly cool them immediately after the processing. The test specimens after the compression test were cut along the longitudinal direction (compression direction) and chemical polishing was performed. In a field emission-scanning electron microscope (FE-SEM), the electron back scattered diffraction (EBSD) pattern was measured at the center of each polished surface. From the measured EBSD data, grain boundaries whose common axes and rotation angles between neighboring crystal grains were within 5 degrees from those of the twinning systems in hexagonal close-packed (HCP) metal were defined as twin boundaries and twinning systems operated at each temperature were analyzed.

3. Experimental Results

Figure 2[5] shows the images of crystal orientation distribution in the compression direction on the test specimens compressed by 10% strain at 25°C, 300°C, and 500°C along with twin boundary distribution. **Table 1** shows the rotation angles and common axes of twinning systems that operated during the 10% compression deformation. In the twin boundary distribution images in Fig. 2, the boundaries having an ideal crystal orientation rotation relationship (error within 5 degrees) shown in Table 1 are colored as twin boundaries. At all the temperatures, twins were formed during the compression deformation. Although four types of twinning systems were observed in this study, the number of formed twins and the active twinning systems vary depending on the deformation temperature. In the test specimen after the compression deformation at 25°C, many small twins were formed, and crossings of the twins and twins in other twins (secondary twins) can also be observed. As active twinning systems, three types of $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, and $\{11\bar{2}2\}$ twins were formed. In the test specimen after the compression deformation at 300°C, although the number is slightly smaller than that at 25°C, twins were still formed at high frequency, and crossings of the twins and secondary twins are observed. The active twinning systems are only $\{10\bar{1}2\}$ and $\{11\bar{2}2\}$ twins, and no $\{11\bar{2}1\}$ twins are seen. In the test specimen after the compression deformation at 500°C, the number of formed twins is even smaller; although crossing of twins can be seen, no secondary twins were formed. The active twinning systems differ from those at lower temperatures, and new $\{10\bar{1}1\}$ twins are observed, in addition to $\{10\bar{1}2\}$ twins.

Table 2[5] shows the temperature ranges in which the twinning systems were observed in the 10%-compressed test specimens (polycrystals). The temperature ranges in which twinning systems were observed in single crystals[3] reported in the past are also shown. The table shows that, in the polycrystals, the $\{10\bar{1}2\}$ twins operated in the entire temperature range from 25°C to 800°C, while the $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$ twins operated at rather lower temperatures: The $\{11\bar{2}1\}$ twins operated at 200°C or lower, and the $\{11\bar{2}2\}$ twins operated at 400°C or lower. Meanwhile, the $\{10\bar{1}1\}$ twins operated at rather high temperatures at 400°C or higher. In addition, compared to the results of the single crystals,[3] the formation of $\{10\bar{1}2\}$ twins was not reported in the single crystals at 500°C or higher, while in the polycrystals, the $\{10\bar{1}2\}$ twins operated in the entire temperature range from 25°C to 800°C. While the formation of $\{11\bar{2}1\}$ twins was not reported in the single crystals, the $\{11\bar{2}1\}$ twins in the polycrystals operated in the temperature range from 25°C to 200°C. The $\{11\bar{2}2\}$ twins in the polycrystals operated at slightly higher temperatures compared to the single crystals. Although it is not possible to make a general comparison because of differences in chemical composition, strain rate, compressive strain, and other factors, these three types of twins tend to act in polycrystalline materials over a wider temperature range than in single crys-

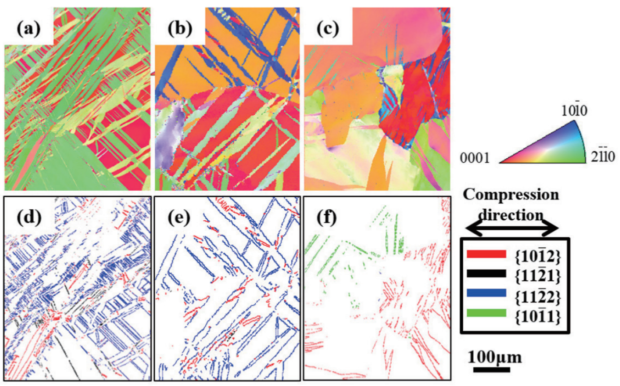

Fig. 2 (a)–(c) Crystal orientation distribution maps of compression directions and (d)–(f) twin boundary distribution maps for specimens compressed by 10% strain at 25°C, 300°C, and 500°C[5]; deformation temperatures are (a) and (d) 25°C, (b) and (e) 300°C, (c) and (f) 500°C. Red, black, blue, and green solid lines in (d)–(f), respectively, indicate $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, $\{11\bar{2}2\}$, and $\{10\bar{1}1\}$ twin boundaries.

Table 1 Twinning systems observed in this study; rotation angle and common axis of each twinning system are also shown

Twinning system	Rotation angle	Common axis
$\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$	95°	$\langle 11\bar{2}0\rangle$
$\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$	35°	$\langle 10\bar{1}0\rangle$
$\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$	64°	$\langle 10\bar{1}0\rangle$
$\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$	58°	$\langle 11\bar{2}0\rangle$

Table 2 Temperatures at which each twinning system was operated for single crystal[3] and polycrystal materials[5]

	$\{10\bar{1}2\}$	$\{11\bar{2}1\}$	$\{11\bar{2}2\}$	$\{10\bar{1}1\}$
Polycrystal (this study)	25°C ≤ T ≤ 800°C	25°C ≤ T ≤ 200°C	25°C ≤ T ≤ 400°C	400°C ≤ T ≤ 800°C
Single crystal[3]	25°C ≤ T < 500°C	None	25°C ≤ T ≤ 300°C	400°C ≤ T ≤ 800°C

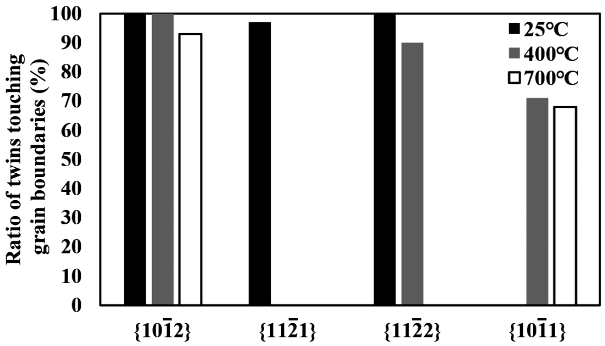

Fig. 3 Ratio of number of primary deformation twins touching grain boundaries to total at 25°C, 400°C, and 700°C

tals. Meanwhile, {10$\bar{1}$1} twins were formed from 400°C to 800°C in both single crystals and polycrystals, so they operate in the same temperature ranges.

Figure 3 shows the results of measuring ratios of the number of the primary twins where any edge of a twin is in contact with a grain boundary to all the primary twins. The figure shows that almost all the {11$\bar{2}$1} twins are in contact with grain boundaries at 25°C. Almost all the {11$\bar{2}$2} twins are also in contact with grain boundaries at 25°C as is the case with the {11$\bar{2}$1} twins, while the ratio lowers to approximately 90% at 400°C. Almost all the {10$\bar{1}$2} twins are in contact with grain boundaries at 25°C and 400°C as is the case with the {11$\bar{2}$2} and {11$\bar{2}$1} twins, while, at 700°C or higher, the ratio lowers to approximately 90%. These tendencies indicate that the concentration of stress and strain near grain boundaries is strongly related to the operation of the twinning systems, and when the temperature is high, such influence is slightly smaller. On the other hand, the ratios of the {10$\bar{1}$1} twins that are in contact with grain boundaries are rather smaller at 70% both at 400°C and 700°C, which may show that the influence of grain boundaries on the operation of {10$\bar{1}$1} twins is smaller compared to the other types of twinning systems.

4. Consideration

In face centered cubic (FCC) metals with good symmetry, because the atoms can move to mirror symmetric positions with twinning planes by uniform shear, twinning deformation completes only by uniform shear deformation. In such a case, twinning systems with small shear strain tend to operate. However, in HCP metals like titanium, twinning deformation cannot be completed by uniform shear alone, and thereby atom shuffling is required to realize the correct orientation relationship of twins.[6] **Figure 4**[7] illustrates the uniform shear and shuffling of a {10$\bar{1}$1} twin, as an example. As shown in Fig. 4 (a), not all the lattice points move to the mirror symmetric positions with the matrix only by the uniform shear (red circles and red crosses). Therefore, shuffling shown with the blue arrows in Fig. 4 (b) is necessary. Generally, in twinning deformation requiring shuffling, twinning systems for which the number of atoms to be shuffled and their moving distance are smaller tend to operate. The shuffling parameter (q) is an indicator to simply show the difficulty of shuffling. The shuffling parameter is the number of crossing times of the minimum lattice vector (translational symmetry vector) parallel to the η_2 (conjugate shear direction) in the twinning system shown in **Fig. 5** over the planes that are parallel to twinning plane K_1. By using Fig. 4 as an example, the aforementioned translational symmetry vector (green arrow) crosses eight planes parallel to the twinning plane, and therefore the shuffling parameter of a {10$\bar{1}$1} twin is eight. Accordingly, the difficulty of operation of twinning systems in HCP metals depends on the shuffling parameter: Twinning systems with a smaller parameter tend to be more active.

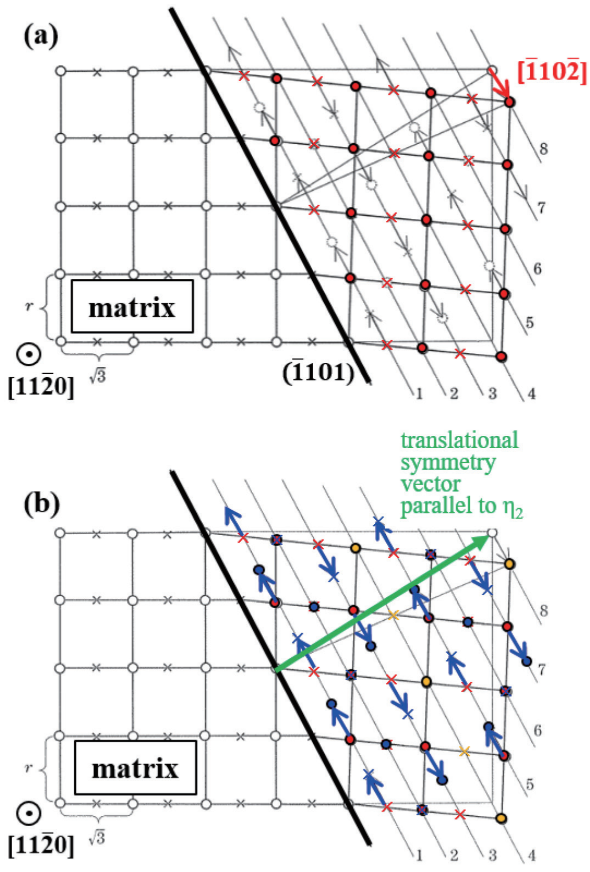

Fig. 4 Schematic diagram of uniform shear deformation and shuffling for {10$\bar{1}$1} twin[7]
(a) after uniform shear deformation, (b) after shuffling
○ and × in the figure indicate lattice points that are offset by a/2 in the vertical direction to the sheet, respectively.

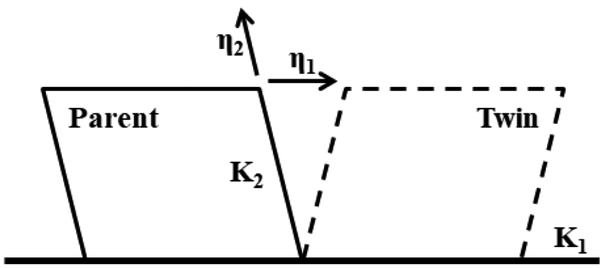

Fig. 5 Crystallographic elements of twinning

Table 3[8] shows the shear strain (s) and shuffling parameter (q) of the twinning systems observed in this study. For the {10$\bar{1}$2} twins that operated in the entire temperature range, the shear strain is the second smallest among the observed twin types and the shuffling parameter is also the second smallest. For the {11$\bar{2}$1} twins that were formed at rather lower temperatures at 200°C or lower, the shuffling parameter is the smallest and the shear strain is the largest. For the {11$\bar{2}$2} twins that were observed at rather low temperatures

Table 3 Shear strain (s) and shuffling parameter (q) in each twinning system[8)]

Twinning system	Shear strain (s)	Shuffling parameter (q)
$\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$	0.174	4
$\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$	0.630	2
$\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$	0.219	6
$\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$	0.099	8

and the formation temperature range was larger for the polycrystals than that for the single crystals, the shear strain is the second largest and the shuffling parameter is also the second largest. The shear stress of all three types of twins above is approximately two times or more than that of the $\{10\bar{1}1\}$ twins whose shear stress is the smallest. For the operation of twin dislocations, large shear stress needs to be applied. As shown in Fig. 3, almost all the $\{10\bar{1}2\}$, $\{11\bar{2}2\}$, and $\{11\bar{2}1\}$ twins are in contact with grain boundaries. From these, $\{10\bar{1}2\}$, $\{11\bar{2}2\}$, and $\{11\bar{2}1\}$ twins may be caused by stress/strain concentration generated near grain boundaries during deformation. Therefore, such twinning systems may be rather easily generated in polycrystals that tend to cause such stress concentration. As shown in Table 2, the $\{11\bar{2}1\}$ twins operated only in the polycrystals, and the $\{10\bar{1}2\}$ and $\{11\bar{2}2\}$ twins operated in a wider temperature range in the polycrystals than in the single crystals. These experimental results match the aforementioned consideration without contradiction.

Meanwhile, although the shear strain of the $\{10\bar{1}1\}$ twins that operated only at high temperatures is the smallest among the four types of the twinning systems, the shuffling parameter is the largest. The elementary process of shuffling when twins are operating has not been clarified, but vacancies, lattice vibration, diffusion, and other factors may influence because it is a movement of lattice points (atoms). Therefore, shuffling may easily occur at high temperatures compared to room temperature. That is to say, $\{10\bar{1}1\}$ twins for which many atoms need to shuffle over long distances may not be formed at low temperatures and operated only at high temperatures (400°C or higher in this study), at which shuffling occurs easily. On the other hand, the shear strain of the $\{10\bar{1}1\}$ twins is very small. That is to say, the shear stress required for movement of twin dislocations is small for $\{10\bar{1}1\}$ twins, and stress concentration is not always required for the formation unlike other types of twins. For these reasons, the active temperature ranges are not different between single crystals and polycrystals for $\{10\bar{1}1\}$ twins. As described above, although it seems at first that twinning systems formed in titanium change in a complicated way depending on the deformation temperature range, it is found that the behavior can be explained in a very reasonable manner by considering the contribution of shear stress and temperature to the shear strain and shuffling parameters.

5. Conclusion

The JIS Class 1 polycrystalline commercially pure titanium materials were uniaxially compressed at 25°C to 800°C and the active twinning systems were investigated. The following conclusions were obtained.

(1) The $\{10\bar{1}2\}$ twins operated during the compression deformation in the entire temperature range from 25 to 800°C. Meanwhile, the $\{11\bar{2}1\}$ and the $\{11\bar{2}2\}$ twins operated at low temperatures: The $\{11\bar{2}1\}$ twins operated from room temperature to 200°C, and the $\{11\bar{2}2\}$ twins operated from room temperature to 400°C. The $\{10\bar{1}1\}$ twins operated only at high temperatures at 400°C or higher.

(2) While the temperature ranges in which the $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, and $\{11\bar{2}2\}$ twins were formed are wider in the polycrystals than in the single crystals, the $\{10\bar{1}1\}$ twins were formed in the same temperature range in both polycrystals and single crystals.

(3) For the twinning systems that were formed by 10% compression at 25°C to 800°C, the ratios of primary twins that were in contact with grain boundaries to the entire primary twins were 90% or more for the $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, and $\{11\bar{2}2\}$ twins, while the ratio for the $\{10\bar{1}1\}$ twins was rather small at approximately 70%.

(4) $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, and $\{11\bar{2}2\}$ twins, for which the shear strain required for twinning deformation is rather large and shuffling is rather easy, require stress concentration at grain boundaries to operate. Meanwhile, $\{10\bar{1}1\}$ twins, for which the shear strain is the smallest and shuffling is most difficult, occur only at high temperatures at which shuffling is easy.

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