Research Article

Experimental Study on Formation Characteristics and Laws of Dislocation and Stacking Fault during Cutting of Titanium Alloy

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Formation characteristics and laws of dislocation and stacking fault during cutting of titanium alloy were investigated by TEM. Several crucial aspects of experiment, such as sample cutting, mechanical reduction of thickness, dimpling, and ion reduction of thickness, were carefully designed and implemented. Further, electron diffraction pattern, diffraction contrast image, and high resolution electron photomicrograph of α phase and β phase were observed and analyzed. Following those analyses, the formation characteristics and laws of dislocation and stacking fault were made clear. Research results show that the edge dislocations exist commonly in the diffraction contrast images and high resolution electron photomicrographs of α phase and β phase. The stacking fault energy is higher in β phase than in α phase. In addition, the extended dislocation is difficult to be seen in β phase, but it is easier to be produced in α phase.

1. Introduction

Titanium alloys, specifically Ti6Al4V, are used widely in aerospace industry, which offer favorable mechanical characteristics such as high strength-to-weight ratio, toughness, superb corrosion resistance, and biocompatibility [1, 2]. But titanium alloys are also difficult to machine materials with considerable manufacturing problems [3]. The distortion of titanium alloy thin-walled part due to CNC machining is one of the most striking process problems that exist in the manufacturing process of aerospace parts [4–8], which greatly impacts the production quality and efficiency and also leads to great economic losses.

Previous researches have shown that when metal crystal is under force, the dislocation (line defect) inside of the metal crystal massively proliferates and causes a lot of crystallographic plane (slip plane) movement, which results in plastic deformation of material [9, 10]. Considering the fact that the machining distortion of titanium alloy thin-walled part is a kind of significant plastic deformation mechanical behavior, the machining distortion is closely related to the geometry form and movement of dislocation. Cutting of titanium alloy is a process with exceeding nonlinear and heat-stress coupled [11]. Within the material, some atoms deviate from

their ideal locations under the influence of heat and stress, resulting in the crystal defects, and as a consequence, the various material properties are inevitably influenced. Further researches show that the perfect dislocations decompose under the action of thermal stress and extend a piece of stacking fault (planar defect) between two partial dislocations [12]. This kind of planar defect not only reflects the way how perfect dislocations decompose but also relates closely to the mechanical properties of material itself. Therefore, researches of dislocation and stacking fault are significantly helpful to reveal the essence and mechanism of the machining distortion for titanium alloy thin-walled part and will also provide a theory basis for controlling machining distortion.

At present, there are a large amount of dislocation theory and experiment researches both at home and abroad. H. Wei and Y. Wei [13] investigated the impingement of a screw dislocation on intrinsic stacking fault (SF) and extrinsic stacking faults (ESF) in different FCC metals by using the molecular dynamics simulations, which were significant to further understand the details of plastic deformation and to seek the underlying techniques for strengthening metals; Dey et al. [14] studied microstructure parameters of plastically deformed (hand filed) Cu–1Sn–Zn ternary alloys with zinc

FIGURE 1: Cutting experiment process.

FIGURE 2: Dimpling process.

FIGURE 3: Ion reduction of thickness process.

concentration 10–24 wt.% with X-ray diffraction line profile analysis; Nakai et al. [15] investigated the grown-in defects in CZ-Si crystals grown at the rate of 0.4 mm/min by bright field IR laser interferometer and transmission electron microscopy (TEM). Their researches concluded that the stacking fault was formed by the agglomeration of self-interstitial atoms during crystal growth; Meng et al. [16] reported direct observation of the formation of threading dislocations from stacking faults in GaN layers grown on (0 0 0 1) sapphire by hydride vapor phase epitaxy; Huang et al. [17] studied the structural stability and generalized stacking fault energies of the $\{1\ 1\ 2\}$, $\{1\ 1\ 1\}$ and $\{1\ 1\ 0\}$ $\{1\ 1\ 1\}$ slip systems in β Ti-Nb alloys with various valence electron numbers; Yang et al. [18] carried out compression tests of Cu-2.2 wt% Al, Cu-4.5 wt% Al, and Cu-6.9 wt% Al with different stacking fault energy and investigated the effect of stacking fault energy upon Cu-Al alloys. Combining that with the existing work, although there are a lot of dislocation and stacking fault studies, research of dislocation and stacking fault during cutting of titanium alloy thin-walled part is rarely reported at the present.

In this paper, taking Ti6Al4V titanium alloy as research object, based on electron diffraction and contrast imaging theory, the transmission electron microscopy (TEM) was used to investigate the formation characteristics and laws of dislocation and stacking fault during cutting of titanium alloy thin-walled part. With the observations and analysis of electron diffraction pattern, diffraction contrast image and high resolution electron photomicrograph, the formation characteristics and laws of dislocation and stacking fault were obtained.

2. TEM Experiment

2.1. Experimental Materials and Cutting. The experimental material was Ti6Al4V titanium alloy after annealing heat treatment, the dimensions of which in length, width, and height directions were 50, 50, and 10 mm, respectively. The hardness of material was about 34 HRC. The chemical compositions of material are shown in Table 1 and the mechanical and thermal physical properties are shown in Table 2.

Cutting of titanium alloy was conducted with the DHF UTJ1004 milling cutter. The cutting parameters

used in experiment were given, including the feed speed 300 mm/min, the radial cutting width 2 mm, the depth of cutting 3 mm, and the spindle rotation speed changed in the range of 800–1500 r/min. The cutting process is illustrated in Figure 1.

2.2. Sample Preparation

(1) *Sample Cutting.* The titanium alloy workpiece was sampled using CNC EDM wire-cut machine tools of DK7750 type and was cut into thin slices of about $10 \times 10 \times 0.5$ mm.

(2) *Mechanical Reduction of Thickness.* The sample was cleaned with acetone for 3~5 minutes. After the sample was naturally dried, the sample holder was heated at 135°C for 5~10 minutes; then the sample was fixed on the sample holder using paraffin and placed in grinding plate. The sample was grinded manually to about 150 microns with “8-” shaped trace on abrasive paper (superscript no. 500); then the sample was cleaned by water and dried and polished with abrasive paper (superscript no. 1000). At last, the sample was removed from the heater and cleaned with acetone for 2 minutes. Similarly, the other side of sample was pasted on sample holder using paraffin, and the mechanical reduction of thickness was carried out according to the previous actions.

(3) *Dimpling.* With diamond grinding paste and phosphor copper wheel, the sample was finely grinded further using the Gatan 656 ultra-precision dimpling grinder. Then the sample

FIGURE 4: Calibration process of α phase structure analysis for titanium alloy. FIGURE 5: Calibration process of β phase structure analysis for titanium alloy. FIGURE 6: Double-beam approximate bright contrast images of α phase.

TABLE 1: Chemical compositions of Ti6Al4V titanium alloy (mass fraction/%).

Al	V	Fe	O	C	N	H
5.5–6.75	3.5–4.5	0.3	0.2	0.1	0.05	0.015

TABLE 2: Mechanical and thermal physical properties of Ti6Al4V titanium alloy.

Temperature/°C	20	250	400	600	700	800	850
Elastic modulus/GPa	125	110	100	74	55	27	5
Yield stress/MPa	803.89	701.32	605.32	500.82	462.1	397.12	321.37
Thermal expansion coefficient/ $10^{-6}/^{\circ}\text{K}$	8.78	9.83	10.68	11.42	12.01	12.21	12.37
Thermal conductivity/W/m·K	6.8	8.7	10.3	13.72	16.23	17.31	17.86
Specific heat/J/Kg·K	611	653	691	749.3	812.4	896.3	932.5

FIGURE 7: High resolution electron photomicrograph with extended dislocation in α phase.

was polished using the felt wheel and was thinned to about 20~30 microns, in which the Al_2O_3 suspension was taken as polishing liquid. Figure 2 shows the dimpling process.

(4) *Ion Reduction of Thickness.* Ion reduction of thickness process was conducted with Gatan 691 PIPS instrument. The sample was cleaned and dried; then it was glued to the molybdenum ring with diameter of 3 mm. After that, the sample was cured by heating at 60–100°C for 10 minutes; then it was put in the sample room of instrument. At last, the sample was thinned to below 50 microns, so it can be penetrated by transmitted electron. Figure 3 shows the ion reduction of thickness process.

The sample prepared was investigated by TEM. The experiment instrument was CM200FEG high resolution transmission electron microscopy and the parameters were used, including the working voltage 200 kV and the point resolution 0.24 nm.

3. Results Analyses

3.1. *Phase Structures Analyses.* Titanium alloy belongs to dual-phase material and its phase structure can be determined by diffraction pattern. Based on TEM

experiment results, the observation area was fixed with district aperture, and the diffraction spots behind focal plane were enlarged, thus forming clear high resolution electron photomicrograph. The calibration processes of phase structures analyses for titanium alloy are shown in Figures 4 and 5.

According to the commonly used diffraction spectrum of different crystal structures, the distance of crystal face was calculated and the crystal structure was determined. The calculating formula is given by the following equation:

$$L\lambda = Rd, \quad (1)$$

where L is the distance between the sample to the baseboard, and its value is 470 mm; λ is the wavelength of the incident beam, and its value is 0.0256 Å; R is the distance between diffraction spot and transmission spot; d is the distance of crystal face; R can be measured directly using ruler on the electron diffraction pattern film. For Figure 4, R_1 and R_2 are 4.67 mm and 4.025 mm, respectively. For Figure 5, R_1 and R_2 both are 4.37 mm. d is calculated according to (1). For Figure 4, d_1 and d_2 are 2.576 Å and 2.989 Å, respectively. For Figure 5, d_1 and d_2 both are 2.753 Å.

On the other hand, the distances of crystal faces of two groups of high resolution electron photomicrographs were measured using Digital Micrograph software. For Figure 4, the distance of crystal face (0111) d_1 is 2.235 Å; the distance of crystal face (1010) d_2 is 2.586 Å. For Figure 5, d_1 and d_2 both are 2.25 Å.

At the same time, the distances of crystal face can also be calculated by the existing mathematical model. For α phase (dense-hexagonal structure), the distances of crystal faces are calculated with the following mathematical model:

$$d = \frac{1}{\sqrt{(4/3a^2)(h^2 + hk + k^2) + (l^2/c^2)}}, \quad (2)$$

where h , k , and l are relatively prime numbers a and c are grating constants, for α phase, a is 0.295 nm and c is 0.468 nm. According to this mathematical model, the distances of crystal faces d_1 and d_2 are 2.24 Å and 2.55 Å, respectively.

FIGURE 8: High resolution electron photomicrograph of dense-hexagonal structure.

FIGURE 9: Double-beam approximate bright contrast image of β phase.

For β phase (body-centered cubic structure), the distances of crystal faces are calculated with the following mathematical model:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}. \quad (3)$$

For β phase, a is 0.331 nm. According to this mathematical model, the distances of crystal faces d_1 and d_2 both are 2.34 Å.

Based on the above analysis, it can be seen that the distances of crystal faces obtained from three kinds of methods are relatively consistent. Further, according to the distances of crystal faces, through comparison with reference value of particular crystal structure, the phase structure of titanium alloy can be determined, which is used to analyze the formation characteristics and laws of dislocation and stacking fault during cutting of titanium alloy.

3.2. Dislocation and Stacking Fault Analyses. Interference-free imaging was carried out with the objective aperture trapping single beam transmission light, and the diffraction contrast image was obtained, which could reflect the scattering capacity difference in different areas of the samples. By trapping the transmission spots on back focal plane using objective aperture, the bright contrast image was gained, which was much clearer and can preferably reflect the characteristics of the material morphology.

FIGURE 10: High resolution electron photomicrograph of body-centered cubic structure.

Double-beam approximate bright contrast images of α phase were obtained by trapping the transmission spots of diffraction pattern in Figure 4 with objective aperture. The bright contrast images are shown in Figure 6.

Dislocations move along the slip plane under the action of shear stress. When stopped by the barriers, these dislocations pile up before obstacles, such as grain boundary or large size precipitation, and form regular arrays, which are called dislocation pile-up. In Figure 6, label 1, label 2, and label 3 are the dislocation pile-up of different forms, and label 4 is grain boundary. When the number of dislocation pile-up reaches a certain level, it can make the dislocation source of neighboring grain move and cause great stress concentration for leading dislocation at the forefront, which leads to plastic deformation or crack initiation. Under a sustained effect of deformation, the tiny crack grows up gradually, and when it goes over critical size, the macrodamage is triggered.

The lower stacking fault energy makes it more possible to generate dislocation pile-up and makes the moving perfect dislocations in alloys decompose partial dislocations more easily. A piece of stacking fault can be extended between two partial dislocations, which takes the shape of fringe contrast under the electron microscope. The attached partial dislocation and stacking fault at both ends are collectively described as extended dislocation.

The high resolution electron photomicrograph of the sample was investigated and extended dislocation was found in α phase. Corresponding to fringe contrast of bright contrast image, the extended dislocation is shown in Figure 7.

In Figure 7, the Burgers vector of the stacking fault (SF) is $(1/3)\langle 2\bar{1}10 \rangle$. In addition, there is half of the dislocation at both ends of SF (as indicated in the figure by the arrow) and their Burgers vectors are $(1/3)\langle 1\bar{1}00 \rangle$ and $(1/3)\langle 10\bar{1}0 \rangle$ respectively.

Comparison between Figures 6(a) and 6(b) shows that just some dislocation forms without obvious regularity, in which label 1 is grain boundary. These dislocation forms exist commonly in the diffraction contrast images and high

resolution electron photomicrographs and most of them are edge dislocations lacking semiatomic plane.

High resolution electron photomicrograph of dense-hexagonal structure is shown in Figure 8.

In Figure 8(a), there are three dislocations marked as D_1 , D_2 , and D_3 , respectively. Extra semiatomic planes of dislocations D_1 and D_2 embed from the left side, while extra semiatomic plane of dislocation D_3 embeds from the right side. In Figures 8(b) and 8(d), dislocations D_1 and D_3 are magnified and the corresponding Burgers circuits are marked. Burgers vectors of dislocations D_1 and D_2 are in the same direction, but Burgers vectors of dislocation D_2 are not right above dislocation D_1 , which cannot form a balanced structure, so the interaction force between them is a repulsive force. Burgers vectors of dislocations D_1 and D_3 are in the opposite direction and they are not in the same slip plane, so a balanced structure can be formed. Burgers vectors of dislocations D_1 , D_2 , and D_3 are all $\langle 2\bar{1}10 \rangle$.

Double-beam approximate bright contrast image of β phase was obtained by trapping the transmission spots of diffraction pattern in Figure 5 with objective aperture. The bright contrast image is shown in Figure 9. In this figure, label 1 is grain boundary and label 3 is equal inclination fringe.

High resolution electron photomicrograph of body-centered cubic structure is shown in Figure 10.

In Figure 10(a), there are two dislocations marked as D_1 and D_2 , respectively. Extra semiatomic plane of dislocation D_1 embeds from the left side, while extra semiatomic plane of dislocation D_2 embeds from the right side. In Figures 10(b) and 10(c), dislocations D_1 and D_2 are magnified and the corresponding Burgers circuits are marked. Burgers vectors of dislocations D_1 and D_2 are both $(1/2)\langle 111 \rangle$.

Due to the fact that β phase belongs to body-centered cubic structure, it has more slip systems than α phase which belongs to dense-hexagonal structure. When cutting titanium alloy, dislocations in β phase move more intensely and are easier to cause plastic deformation. In addition, because the slip is easier to be produced in β phase, the extended dislocation is difficult to be seen, which reflects that the

stacking fault energy is higher in β phase than in α phase. On the contrary, because the atoms in α phase have a lot of derangement forms, the extended dislocation is easier to be produced in α phase than in β phase.

4. Conclusions

(1) The research results show that the edge dislocations exist commonly in the diffraction contrast images and high resolution electron photomicrographs of α phase and β phase for titanium alloy. The stacking fault energy is higher in β phase than in α phase. Dislocations in β phase move more intensely and are easier to cause plastic deformation. In addition, the extended dislocation is difficult to be seen in β phase, but it is easier to be produced in α phase.

(2) This work identifies the formation characteristics and laws of dislocation and stacking fault during cutting of titanium alloy, which is significantly helpful in revealing the essence and mechanism of machining distortion for titanium alloy thin-walled part.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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