Calculation of microstress in machining distortion of titanium alloy monolithic component based on x-ray diffraction experiment

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Abstract

Machining distortion of titanium alloy monolithic component is closely related to the internal stress of material. In this paper, the various factors causing width effects of X-ray diffraction line were analysed, and the effect of stacking fault on diffraction spectrum was excluded according to the result of TEM experiment. The true diffraction spectrum, which can reflect inside information of Ti6Al4V titanium alloy, was determined using MDI JADE peak shape analysis method. Further, the calculation model of microstress was constructed. Combining with the result of X-ray diffraction experiment, microstress in machining distortion of titanium alloy monolithic component was calculated. This work establishes the foundation for investigating the mechanism of machining distortion of titanium alloy monolithic component.

Keywords: titanium alloy, machining distortion, microstress, diffraction line width effect

1 Introduction

Titanium alloys, specifically Ti6Al4V, are used widely in aerospace industry, which offer favourable mechanical characteristics such as high strength-to-weight ratio, toughness, superb corrosion resistance and bio-compatibility [1, 2]. But titanium alloys are also difficult-to-machine materials with considerable manufacturing problems [3]. The distortion of titanium alloy monolithic component due to CNC machining is one of the most striking process problems that exist in the manufacturing process of aerospace parts [4, 5], which greatly impacts the production quality and efficiency and also leads to great economic losses.

During machining process, cutting force, heat, clamping force and initial residual stress in blank cause machining distortion together. While initial residual stress and machining stress are the root reasons leading to machining distortion. So, study on the internal stress is helpful to reveal the machining distortion mechanism of titanium alloy monolithic component [6-8].

According to stress classification method presented by Macherauch, the internal stress can be divided into three categories [9]:

1) the first class internal stress, that is called macro residual stress, contains large numbers of small grains. When the balance between the first class internal stress is broken, the macro dimension change must be caused;

2) the second class internal stress, that is called microstress. When the balance between the second class internal stress is broken, the macro dimension change can also be caused;

3) the third class internal stress. When the balance between the third class internal stress is broken, the macro dimension change will not be caused.

At present, the researches of macro residual stress are relatively complete, and the measurement methods are also more complete [10-12]. But relatively few researches of microstress have been reported. In this paper, to obtain a more general understanding on machining distortion, the microstress was studied deeply. The titanium alloy Ti6Al4V monolithic component was taken as research object, and the calculation model of microstress was constructed.

2 Calculation model of microstress

When the internal stress exists in the polycrystalline material, the strain must also exist internal strain corresponding, which causes the local distortion and results in changes of its internal structure. These changes are reflected in the diffraction spectrum line, and microstress can be measured by analysing these diffraction informations [13, 14].

By measuring the diffraction line half height to width, and other factors to cause diffraction line widths after separation, it can measure the size of the micro internal stress, which is the theoretical basis of the micro internal stress measurement.

Assuming that diffraction line width is only micro an effect factors, then, assumes that a Crystal surface spacing for d_0, due to micro internal stress of role,

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makes the Crystal surface of surface spacing and d_0 has some deviated, assuming that *d*+ and *d*- respectively with the material diffraction line width half tall in the diffraction Angle 2θ and 2θ, the mean value of the microstrain average is:

$$\varepsilon_{average} = \left(\frac{\Delta d}{d}\right)_{average} \quad (1)$$

and due to $\Delta 2\theta = 2\theta_+ - 2\theta_0 = 2\theta_0 - 2\theta_-$, there is:

$$\beta_{hkl} = 4\Delta\theta, \quad (2)$$

where β_{hkl} is the diffraction linear half maximum strength space corresponding full Angle width.

A ray diffraction profile and maximum intensity corresponding to the full width of premises (width). By using the equation:

$$\varepsilon_{\phi\psi} = \frac{d_{\phi\psi} - d_0}{d_0} = -(\theta_{\phi\varphi} - \theta_0)\cot\theta_0. \quad (3)$$

Using relationship with $\frac{\Delta d}{d} = -\cot\theta\Delta\theta$, there is:

$$\left(\frac{\Delta d}{d}\right)_{average} = \varepsilon_{average} = \frac{\beta_{hkl}}{4}\cot\theta_{hkl}. \quad (4)$$

$$\beta_{hkl} = 4\varepsilon_{average}\tan\theta_{hkl}. \quad (5)$$

In the above formula, β_{hkl} is radians, if converted into degrees, there is :

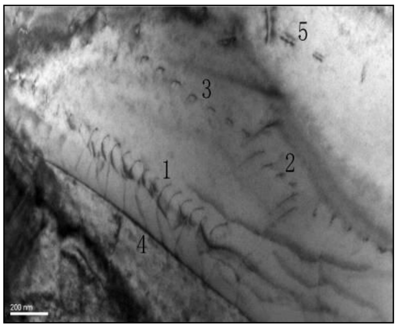
$$\sigma_{average} = E\varepsilon_{average} = E\frac{\pi\beta_{hkl}\cot\theta_{hkl}}{180°\times 4}.$$

The above equation is the calculation model of microstress. But in actual measurement process, instrument etc. system factors, and the crystal block size, stacking fault microscopic internal stress and other materials internal organizational form factors will affect the linear diffraction profiles, the need for specific materials, determine the impact of factors to determine algorithm.

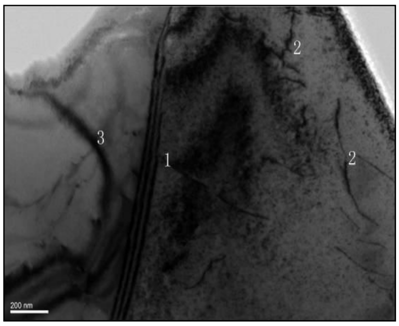
3 Analysis of effect factors of x-ray diffraction line width

3.1 STACKING FAULT OBSERVATION

Experimental material was Ti6Al4V titanium alloy, and the hardness was about 34 HRC. Mechanical thinning (plane grinding), dimpling and ion thinning were performed to achieve the desired TEM sample. The CM200FEG high resolution transmission electron microscopy was used and the microstructure image is shown in Figure 1.



a) Microstructure image along [1213] direction



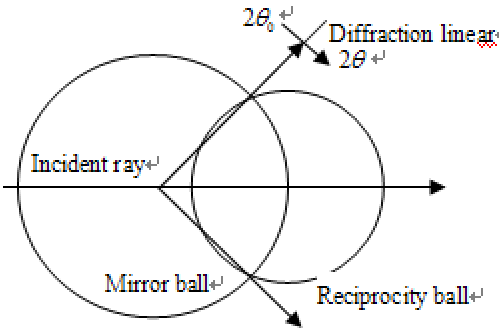
b) Microstructure image along [001] direction

FIGURE 1 Titanium alloy monolithic component after process two-phase microstructure image

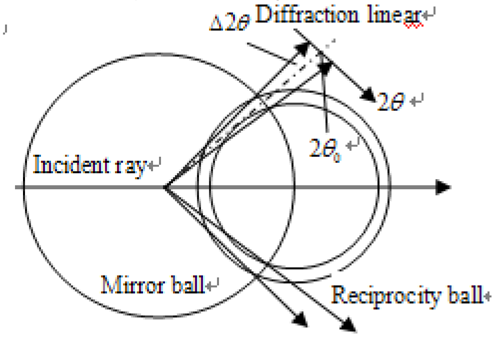
Combining with high resolution electron microscopy image, and Figure 1a identification of 1, 2, 3 place are different forms of dislocation plug product list, 4 place is grain boundary, 5 in dislocation. Figure 1b place 1 for grain boundary, 3 place such as to pour stripe, 2 place two positions for edge dislocation. After observation and analysis, it can be concluded that: Ti6Al4V titanium alloy material cutting internal dislocation motion violent, as dislocation slip one of the main form of the edge dislocation massive exist, in grain boundary place appeared obvious phenomenon of dislocations, and stacking fault there are not obvious. So for diffraction line width influence factors of stacking fault factors, in view of the Ti6Al4V material does not exist, in the follow-up of the solution can be ignored.

3.2 WIDTH EFFECT OF X-RAY DIFFRACTION LINE

For polycrystalline materials, due to the anisotropy, grain size is not the same as. By Edwald graphic method [15], when the crystal block size is relatively large, and each wafer in a crystal plane *hkl* the corresponding reciprocal approximation for a geometric point, cognate surface *hkl* in the numerous crystal block corresponding reciprocal points form a thickness reciprocal ball, as in shown in Figure 2a. And the characteristic of the interference function of analysis, diffractive domain (interference function is not zero area, can be understood as the diffraction ball thickness) of the shape and size of the crystal shape and size of a reciprocal relationship, i.e. material central crystal block size is smaller, diffractive domain is bigger, this resulted in slightly deviated from Prague corner of direction that also exists diffraction, causing diffraction width, as shown in Figure 2b.



a) with the sub-crystal block



b) with the crystal block

FIGURE 2 Diffraction cone schematic diagram

Therefore, the existence of the sub-crystal block for diffraction line width to influence is very serious. Assumption of X-ray diffraction spectrum line width effect separately from the crystal block size factors, well-known German chemist Debye and his graduate student Scherrer is deduced the Scherrer formula can be used for calculation of the crystal block width effect, and the single crystal and polycrystalline are applicable.

$$D_{hkl} = \frac{0.89\lambda}{\beta_{hkl}\cos\theta_{hkl}}, \tag{7}$$

where $D_{hkl} = Nd_{hkl}$ is the crystal block size, half tall wide β_{hkl} units for radian.

Based on above research, can determines sub-cystal block size and micro distortion both is effect physical width of main factors, Asia Crystal block size, and micro distortion of judgment method, is through observation the different diffraction orders of the diffraction lines of physical width β, if $\beta\cos\theta$ for constant, is description wide of by Asia Crystal block wide of effect caused, if beta cot θ for constant, is description wide of is by micro distortion caused, if both are not constant is description this two kind of factors common exists, affecting the physical width of the linear .

4 Calculation of microstress

4.1 X-RAY DIFFRACTION EXPERIMENT

In accordance with the principles of calibration samples location and orientation of the selected measurement points, residual stress test use X-ray stress Analyser XSTRESS3000, this instrument use solid linear detector technology, X-rays can be directly converted into electric signal. In order to improve the measurement precision, the larger collimator, Psi (ψ) and Phi (φ) swing and swing method were used.

The four measurement points are designed and shown in Figure 3. By measuring the stress free Ti sample of powder, measurement can be carried out after instrument calibration and the measuring process is shown in Figure 4.

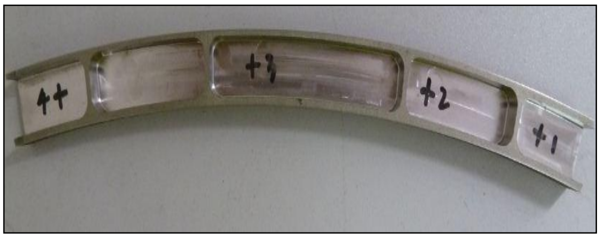


FIGURE 3 Measurement point design

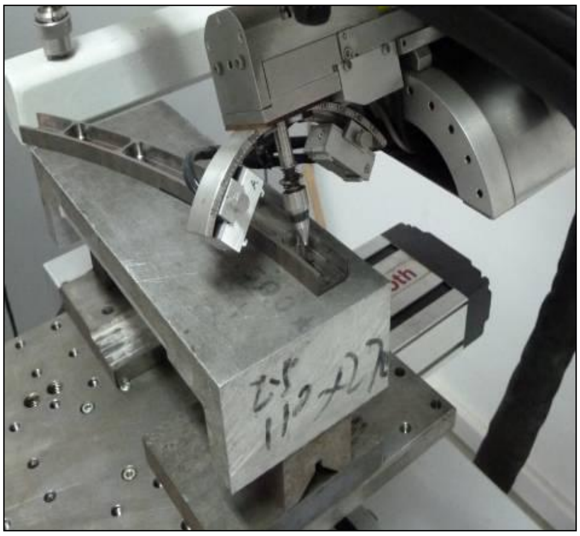


FIGURE 4 Measuring process

4.2 CALCULATION OF MICROSTRESS

The XSTRESS3000 measurement data is converted to MDI JADE procedures to be identified format. Fitting work make up by phase retrieval, deduction of back strength, deduction $K_{\alpha 2}$, deduction of equipment of spectral line widths, as well as for smoothing.

MDI JADE software in the analysis of map is automatically deducted from the instrument width effect with map smooth, get the measurement point of the real diffraction spectra (physical width of spectral lines), is shown in Figure 5.

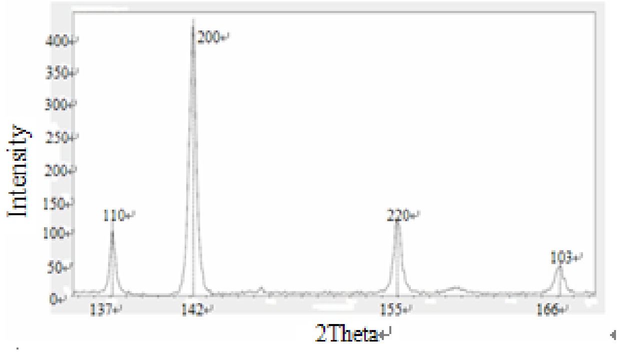


FIGURE 5 Measure point diffraction line (physical width)

For the cognate crystal surfaces 110 and 220, the diffraction peak shape similarity, the half high width β in numerical value is approximately the same, and the 2θangle is quite different, so the crystal block size and microscopic distortion two factors are present. The line width is not only simple mechanical superposition, but a convolution relation, JADE procedures in the convolution process regard the diffraction line approximation as a specific function to solve. Approximate function method is the crystal block width function and microscopic distortion line width function as a known function, such as the Gauss function, Cauchy function or Cauchy square functions etc.

Due to the two kind of line width effect is not a simple mechanical superposition, but they form convolution, so by a line cannot completed. Need to measure two or more than two diffraction peak half high width β, due to the crystal block size and crystal indices related, so the diffraction plane selection to choose the same direction, for example (110) and (220), get of each spectral line width β and physical diffraction angle θ. At this time regard $\frac{\sin\theta}{\lambda}$ as X-axis, identify $\frac{\beta\cos\theta}{\lambda}$ and $\frac{\sin\theta}{\lambda}$ linear relation, with the method of the least squares fit a straight line, the slope of the straight line for micro strain two times, straight line in the ordinate of intercept for crystal block size reciprocal, thus determining the crystal block size D and microscopic distortion ε value.

Using MDI JADE program for data operation processing is as follows:

1) Measurement of specimen on the reverse side one points more than two diffraction peaks, for the same direction secondary diffraction;

2) Reading in data in JADE, for phase retrieval, deduct back bottom strength, deduction and map smooth, full spectrum fitting; into the JADE, for phase retrieval, background subtraction, deduction, as Atlas strength smooth, full spectrum fitting;

3) Checking instrument half tall wide compensate curve is correct, select menu "Report – Size&Strain Plot" instruction, open the calculation dialog;

4) Selecting size/strain, adjust D value to 1.5. If the shape is more closer to the Gauss function, it is set to two, if the shape is more closer to the Cauchy function, take D=1.The value of D size influence single value of the experimental results, for sample regularity there are no influence;

5) Saving the image. Saving calculation results export to text format, calculation results is shown in Figure 6.

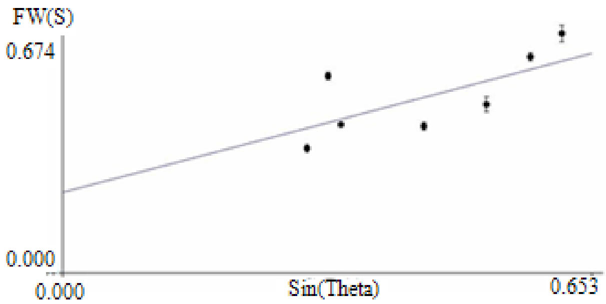


FIGURE 6 Calculation results

In the Figure 6, FW (S) represents the physical width. Strain represents micro strain, as the ratio of train value with the plane spacing, Strain is 0.2461%, the strain value was 0.01638, R represents error. The method of approximate function is the calculation of average grain size, because different crystal face size is not the same, the calculation results represent the direction of each diffraction the size of the grain size. Calculation results of microstress are shown in Table 1.

TABLE 1 Calculation results of microstress

Time node	Measurement points	ε (nm/nm)	σ (MPa)
Machining finished	No.1	0.018306926	211.81
	No.2	0.019924986	230.53
	No.3	0.01614891	186.84
	No.4	0.015250658	176.45
40 days passed	No.1	0.009100099	105.29
	No.2	0.011571049	133.88
	No.3	0.00934011	108.07
	No.4	0.010033111	116.08
80 days passed	No.1	0.012416515	143.66
	No.2	0.014536224	168.18
	No.3	0.016056433	185.77
	No.4	0.012811376	148.23

5 Conclusions

1) The calculation model of microstress in machining distortion of titanium alloy monolithic component was proposed. The premise of calculation is that the diffraction spectrum line must be determined first, and the calculation is a solving process using convolution relationship.

2) The various factors causing width effects of X-ray diffraction line were analysed comprehensively, and the effect of stacking fault on diffraction spectrum was excluded according to the result of TEM experiment. The true diffraction spectrum, which can reflect inside information of Ti6Al4V titanium alloy, was determined using MDI JADE peak shape analysis method.

3) According to calculation model of microstress, combining with the result of X-ray diffraction experiment, the microstress in machining distortion of

titanium alloy monolithic component were calculated.

4) This work establishes the foundation for investigating the mechanism of machining distortion of titanium alloy monolithic component.

Acknowledgments

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