Simulation of Plastic Deformation Behavior of Ti-6Al-4V Alloy by Finite Element Method

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ABSTRACT

Mechanical properties of alloys have a strong relation with microstructure and determination of their behavior can lead to multiple advantages. To obtain this goal, finite element method (FEM) is one of the best ways. In this study a series of experiments were carried out on the produced Ti-6Al-4V to obtain its mechanical characteristics and to prepare it for photographing in micro dimensions. Next, using scanning electron microscopy (SEM), images were taken from some regions of the manufactured Ti-6Al-4V. In the next step, a method was developed to separate alpha-phases from beta-phases with a relatively high accuracy. At the end of this stage, the images were mapped into a matrix involving arrays which show the type of the phases. A code is written which maps the material matrices to the FEM model. The Gurson model is an appropriate model for simulating the damage inside the ductile material. Results of simulations obtained from SEM images show that the simulation data are in good agreement with experimental results and also analysis of simulation clearly shows that the failure always happens in boundaries between two different phases; ductile and brittle, and then growth over them to form the final failure of the material.

1. Introduction

Due to the exclusive and superb properties that titanium alloys show, today they are applied extensively in various industries [1]. The most important properties of titanium include biocompatibility, good resistance to corrosion and fatigue and high ratio of strength to weight. Among the titanium alloys, Ti-6Al-4V alloy is recognized as the most important and applicable titanium alloy [2]. Today instead of practical tests and trial and error methods, using engineering software packages is one of the new techniques for understanding the behaviors of method, so that by optimizing the test results, a model for practical behavior could be obtained by the engineering software packages, to be generalized for similar activities under different conditions. This could prevent losing of materials, time and energy and also will reduce the testing errors [3].

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Since the mechanical properties of alloys depend on their microstructures, developing simulated models seems to be essential for identifying and determining materials behaviors, predicting the alloys properties such as mechanical properties and for defining practical strategies regarding engineering designs [4].

The aim of the present research is developing the simulated model by finite element method in order to obtain the alloy plastic deformation behavior according to the materials microstructures, and compare it with real conditions to obtain the material response to the stimulants such as tension, and use it in designing and performance of the alloy.

2. Materials and research methodology

The Ti-6Al-4V alloy used in this research is a plate with the thickness of 0.7 mm and in annealed form. The chemical composition of this alloy is shown in table (1).

Table 1. Chemical composition of Ti-6Al-4V

Elements	Al	V	С	0	Fe	Н	Ti
wt%	6.3	4	0.1	0.2	0.1	0.05	Bal

Upon microstructural studies, after hot mounting, first the samples undergo mechanical polishing by sand paper (80 to 4000) and then the surface of specimens are polished by diamond paste. After that samples were washed by an ultrasonic device and degreased by acetone. The applied etchsolution is composed of carol solution with the composition of 10 ml of hydrofluoric acid, 5 ml of acid nitric and 85 ml of distilled water. Finally, microstructure evaluation was done by using scanning electron microscopy (SEM) and an optical microscope (OM). The primary microstructure of Ti-6Al-4V can be observed in Fig.1.

X-ray diffraction (XRD) analysis is used for identifying different phases of the alloy. Philips X pert-MPD system (with wavelength of *Cu Ka*equal to 1.542) has been used for this purpose, and the other parameters used for it included the applied voltage of 30 Kv with current of 30 mA, and the diffraction angle (2θ) of 20 to 90°.

The samples were prepared according to ASTM E8M standard for the tension test and underwent the test by HOUNSFIELDH50KS device of the ambient temperature by applying the strain rate of 3×10^{-4} m/min and the pressure of 3 bars.



Fig.1. Microstructure photograph (a)optical microscope (b) scanning electronmicroscope.

Generally, identification of the material behavior by using metal microstructures requires a high accuracy in modeling. The researchers used to use random methods for modeling that could lead to the results with low accuracy. The reason for the error coefficient in simulating results as compared to practical results is that the geometry of particles in microstructural modeling is quite effective in the obtained results. Hence, trying for modeling the material, according to image processing is quite important in simulation of the material [5].

The Gurson damage model that was offered in 1977 and could have acceptable predications for soft materials was used in solving the problem. This model is used for α -phase (soft phase), and the elastic-plastic model is applied for the β -phase, which is a rather harder phase. The simulated model is obtained by analyzing the images, such that primarily, after doing the tensile test, the cracked levels are evaluated by the scanning electron microscope. For modeling from SEM images, the images are taken to MATLAB environment and definition of phases is done by the use of image analysis method. This idea is executed by the total optimized thresholding method, by Otsu technique, and finally the soft phase could be distinguished from the hard phase. To do this, by encoding in MATLAB software and using the RGB color model and forming three color matrices for the considered image; then the separation and distinguishing the color domain that is specific for the pixels is done. This finally leads to separation of the soft phase from the hard phase. [6] It is to say that by increasing the number of image pixels, the phases are separated by higher precision. At the last stage the image is put on a matrix, the arrays of which define the type of the phases, so that the soft phase and the hard phase are attached to the ithrow and jthcolumn of the matrix. This array is made of rectangles and each rectangle is in conformity with the considered material. Finally, a model is made that is similar to the actual image [7].

To follow, the numerical solution and comparison with the empirical results are done by ABAQUS software. The resulted algorithm that is due to writing the software package for analyzing the images considers the following points:

1- Reading SEM images of the Dual-phase alloy (α and β)

2- Identifying the color domain of the obtained image from SEM

3- Distinguishing the phases and separating the boundaries from each other

4- Allocating the material according to the color, to the pixels

5- Writing the resulted matrix of the alloy, in finite element method model

Fig.2 shows the transformation of the obtained results from the SEM images to the finite element model. The image of SEM from alloy is shown in Fig.2a. At first the phases are separated and Fig.2b shows a binary image of them. In this figure the white color represents β -phase. Following that, by writing codes in MATLAB (different to the thresholding method), the share of the color matrix would be allocated to each pixel. Then all the results from MATLAB that include the coordinates and physical properties of all the pixels would be transferred to Python software (to reduce the calculation time). Through encoding in this software, the pixels are placed beside each other in accordance with the geometrical coordinates. Each pixel represents an element, too. Then the model is reticulated, in such a way that the dimensions of the elements are equal to the dimensions of the image pixels. It means that the image pixels are transformed to the model elements in ABAQUS software, by one by one correspondence (Fig.2c).

It is to say that the number and dimensions of the pixels is exactly equal to the number and dimensions of the elements of finite element model. The number of pixels in X and Y coordinates in the above images equals 330 and 265. Two-dimensional elements are used for simulation.

The square elements assigned to the geometrical model are observed in Fig.3. Number of elements has determining roles. Hence, the case should be analyzed for different numbers of elements. 90,000 elements have the proper mapping potentials for the boundary between the phases and provide acceptable results for simulation, in comparison with the practical results [7,8].



Fig.2. Image processing procedure for image (a) SEM image (b) Recognition of phases (white colour is Beta and black colour is Alpha phase) (c) FEM model.



Fig.3. Square element in finite element software.

The repeating boundary conditions will lead repetitive micromechanical to models deformations. It means that if a point is projected on a surface of the micromechanical model, it will have a notch on the other side. This boundary condition is the most accurate condition for simulating stress concentration in microstructures, since it simulates the internal material condition in a proper way. The state of repeating boundary condition will minimize the effects of the constraints. Fig.4a shows the middle part of a component that analysis of its properties is to be considered and Fig.4b is a part of the component in micro-dimensions that is to be considered in simulation. Accordingly, the boundary condition is defined in such a way for the micro particle that lots of them could be placed beside each other to form the component. Different studies show this boundary condition in micro-dimensions and homogenizing the results will provide the best approximation for the macroscopic component behavior [7, 8].



Fig.4. Boundary condition in micro mechanic model (a) in repeated model (b) in the material.

The repeatable boundary condition is applied in X and Y coordinates in modeling. Regular square meshes are used in all the simulations. It is better to note that the geometry is reticulated by the use of square elements. This facilitates the probability of applying repeating boundary conditions with higher precision. For solving this case, the straightforward solver is used in order to use the damage model in case of necessity. In this case, the geometrical boundary condition that is based on displacement (due to shorter solution time as compared to the normal boundary condition) is used. It should be reminded that the loading in simulation is according to the standard of the tension device.

3. Results and Discussion

X-ray diffraction pattern of the alloy is observed in Fig.5. According to this pattern, the forming phases of this alloy are of alphaphase enriched by aluminum and beta-phase enriched by vanadium.



Fig. 5. X-ray diffraction pattern of Ti-6Al-4V.

Fig.6 shows the micrograph of the simulation of the alloy microstructure that the two forming phases are completely separate from each other due to color distinctions, and the inter-phase boundary is a well-defined property. The light areas in this image are the beta-phase and the dark areas are the alpha phase.



Fig.6. Simulated micrograph of Ti-6Al-4V by FEM.

Fig.7 shows the obtained stress-strain curve via the tension test and predicted by the

simulated model. The obtained results show proper conformity between the experimental and simulated data, so that the errors could be neglected.



Fig.7. Stress-strain diagram of experimental and numerical studies.

The simulated states of stress distribution and the cracking method are shown in Fig.8. In part (a) the Von Misses stress is shown for the strain of 2%. In part (b), in strain equal to 10%, the most stress has been in 45° related to the tensile force, which indicates that the material has soft behavior and most of the stress in red color is observed in the areas between the two phases of soft and hard. In the strain of 10% where the void is formed, the material yields at 45° , so that the voids are extended in that direction, and by the expansion of the crack and their connections to each other, the materials will be damaged in dimple form.

Fig.9 shows the place of the crack initiation in the boundary between soft and hard phases. By the growth of the crack, the material will be yielded and this occurs in reality and cracking starts from these areas. Elasticplastic behavior was considered for the hard phase (Beta-phase) and the isotropic hardness was applied for the plastic state. Also the yield stress is predicated as a function of plastic strain. A function of plastic strain is also predicated for the soft phase (Alphaphase).



Fig.8. Simulation of stress distribution (a) Von-Misses stress in 2% strain (b) Von-Misses stress in 10% strain.

In Fig.9, Ti-6Al-4V alloy has undergone a fracture and the dimple effects which are observed on it. Hence, alpha-phase as a soft phase that has considerable flexibility is considered. In contrast to alpha-phase, betaphase has higher hardness, so that it could tolerate high loads with the least deformation. Gurson - Tevergaard - Needleman damage model (offered for soft materials) was used in this research. It provides acceptable results when correct parameters are considered for the soft-phase. Regarding the micrographs showing cleavage and dimple damage indicating the crack formation in the material, it can be concluded that cleavage damage occurs in hard phase, while dimple damage occurs in soft phase. The voids are formed between the two types of damages and develop. It shows that usually a void or crack is initiated at the boundary. Hence, Gurson damage model is used for the soft-phase and Table 2 shows the type of considered finite element specifications.

After the tensile test, fractography was done by scanning electron microscope. Fig.10 shows microscopic image from the fractured surface of the sample. Regarding the images from the sample section after the tensile test, it can be seen that the fractured surface of the sample has ductile fracture specification. Presence of small dimples with 4-10 micrometers diameters on the fractured

surface of the sample indicates the ductile rupture in the material. The presence of the dimples is due to inter-granular cracks occurred at the beginning procedures of By the development deformation. of deformation, the boundary grain cracks become like voids, separation would occur, leading to fractured dimples [9]. When the dimples become smaller, it could indicate the improvement in flexibility of the sample [10]. Presence of dimples with shallow depth and layer plates (flat areas) on the cross-section of the fracture shows low resistance to growth of the crack and low flexibility of the sample [7].



Fig.9. Simulated images from crack initiation and propagation in α/β boundary.

	Material	Hardening Model	Damage model
	Soft phase	Elastic-Plastic	Gurson damage
	Hard phase	Elastic-Plastic	No damage model
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 Table 2.Mechanical model for each phase

Fig. 10. Fractography by SEM.

4. Conclusions

Increasing strain in image analysis method will lead to fractures in materials and damage model has an important role in localization of fractures. Gurson damage model that has acceptable predictions for ductile materials is used in solving the problems. Hence, the damage model is used in this research for the alpha-phase (soft-phase) and the elasticplastic model is used for the beta-phase (hardphase). It should be noted that the structural parameters of damage model are of great importance in conforming the numerical results to the experimental ones. It is clear that emergence of voids occurs in the softphase region. In contrast to the alpha-phase, beta-phase is having a rather higher hardness, so that it could tolerate high loads with the least rate of deformation. It is also to say that emergence of voids occurs near the hard phase and the emergence develops. It could be concluded that development is done at the boundary of two different phases. The experimental and laboratory results confirm the offered mechanism for fractures in Ti-6Al-4V alloy. On the whole, the obtained

results from simulation of plastic deformation of materials by finite element method are quite close to the experimental observations, such as tensile tests and fractographic observations.

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