Finite Element Modeling of Secondary Phase Grain Size on the Stress Strain Curve of Ti alloy

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Abstract—The stress-strain curve of 0.16α of low cost beta (LCB) Ti alloy (Ti–10V–4.5Fe–3Al) was measured and then it was simulated by using finite element method (FEM) based on the individual stress-strain curves of the single-phase α and β, then the measured result compared with the simulated curve. The results showed that the simulated result closely fits with the measured one, which proves that this FEM built in this work is acceptable. This FEM model was used for calculation of stress-strain curve at three different grain sizes at constant volume fraction of α is 16%. The results showed that finer grain size having higher yield strength compared with the coarser one. The results showed that the stress gradient exists in both the phases and the distributions of stress are non-homogeneous. The stress in the α phase is lower than the stress in the β phase, whereas the strain in the α phase is higher than that in the β phase.

Keywords—Grain size, Finite Element Method, Stress-Strain Curve, Titanium alloy.

I. INTRODUCTION

TITANIUM (Ti) alloys having a unique combination of mechanical and physical properties and excellent corrosion resistance to sea water, which make them popular for a variety of applications [1]. Titanium alloys are excellent candidates for aerospace applications owing to their high strength to weight ratio and excellent corrosion resistance [2]. The expansion of titanium applications to non-aerospace industries (e.g., automotive, chemical, energy, marine, biomedical, sports, and architecture) entails improvements in the understanding of titanium metallurgy, advances in processing methods, ability to manufacture components without defects, and development of low cost alloys [3]. Beta titanium alloys offer a wide range of mechanical and chemical properties and can be thermally processed to achieve high strength, toughness and fatigue resistance even in large sections [4]. The development of a low cost beta (LCB) alloy [5] like Timetal LCB (Ti–4.5Fe–6.8Mo–1.5Al) makes use of ferromolybdenum addition to reduce the cost so that it becomes competitive for automobile and other aerospace applications. The alloy possesses excellent workability and mechanical properties which are comparable to that of high strength steel [6].

Mechanical properties of titanium alloys are important criteria of material service capabilities both in aerospace and industrial applications. Microstructure of the alloy is one of the important factors controlling both the tensile strength and the fatigue strength. With different percentages of α and β phases, several metastable microstructures can be formed. Thus, it is formed with integration of several physical properties, functional performances, and strain in different phases and even in different grains is inhomogeneous, it is hard to express the distribution of stress and strain in the titanium alloy clearly [7]. Therefore, any innovation in the design and predicting the properties with the help of microstructure will lead to reduce experimentation and large overall cost savings. The key to these innovations is a thorough understanding of the material’s constitutive response to the imposed conditions and detailed process analysis. This is achieved by effective material modeling and integration of microstructural information with process simulation and optimization methodologies.

Many investigators [8, 9] calculated the stress-strain curve and then compared with the measured one, by using the stress-strain curves of the individual phases. In this paper the stress-strain curve of 0.16α of Ti alloy calculated based on the individual stress-strain curves of single α and β phase alloys using finite element method (FEM). The simulated result was compared with the measured one and then, the distribution of stress and strain of the 0.16α of Ti–10V–4.5Fe–3Al alloy was analyzed in this work. Finally, with the FEM model the effect of secondary phase (α) grain size on the stress-strain curve is calculated.

II. MATERIALS AND METHODS

A. Materials and Methods

The LCB Ti alloy i.e., Ti–10V–4.5Fe–3Al has been used in this work. The chemical composition of the alloy was analyzed using spectrometer and the chemical composition shown in Table 1.

The Ti alloy was produced by using vacuum arc remelting process. The alloy was processed thermo-mechanically in order to get the equiaxed microstructure. Thermo-mechanical process includes forging and rolling. The ingot was forged at 900 ºC (beta forging) in order to remove the defects in the
ingot. Further it rolled into 10mm thick slab at 750 ºC. For microstructural examination, samples were cut from the 10 mm thick slab, and heat treated with the tensile specimens at required conditions, polished metallographically using standard metallographic technique and finally etched with Kroll’s reagent (2ml of HF, 6ml of HNO₃, 92ml of Distilled Water). Etched samples were examined under scanning electron microscopy and optical microscope.

TABLE I. Chemical composition of the Ti-10V-4.5Fe-3Al alloy

<table>
<thead>
<tr>
<th>Elements</th>
<th>V (wt %)</th>
<th>Al (wt %)</th>
<th>Fe (wt %)</th>
<th>O (PPM)</th>
<th>N (PPM)</th>
<th>H (PPM)</th>
<th>Ti</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti-10V-4.5Fe-3Al</td>
<td>9.6-10</td>
<td>3</td>
<td>4 - 5</td>
<td>800</td>
<td>100</td>
<td>19</td>
<td>Rest</td>
</tr>
</tbody>
</table>

The stress-strain curves of single phase α and β are required in order to simulate the stress-strain curve. Hence the stress-strain curve of full β was calculated experimentally and α is taken from the literature [7-8].

TABLE II. Parameters of stress and strain for simulation

<table>
<thead>
<tr>
<th>No</th>
<th>Single Phase α</th>
<th>Single Phase β</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Strain</td>
<td>Stress (MPa)</td>
</tr>
<tr>
<td>1</td>
<td>0.017</td>
<td>296</td>
</tr>
<tr>
<td>2</td>
<td>0.022</td>
<td>318</td>
</tr>
<tr>
<td>3</td>
<td>0.035</td>
<td>341</td>
</tr>
<tr>
<td>4</td>
<td>0.061</td>
<td>349</td>
</tr>
<tr>
<td>5</td>
<td>0.1</td>
<td>355</td>
</tr>
<tr>
<td>6</td>
<td>0.2</td>
<td>369</td>
</tr>
</tbody>
</table>

B. Finite element modeling

From the Fig. 1 it is observed that the α phase is distributed homogeneously on the β phase. A 2D model was built by using FEM replicates the microstructure. The FEM model consists of 800 triangular elements, which are connected by 1681 nodes (Fig. 3). The violet elements represent the α phase, whereas the green elements represent the β phase. The volume fractions of α phase in the microstructure as well as in the FEM model are same of 16%, while remaining is beta phase. Loads are applied in the vertical direction in terms of displacement are as follows: 0.005, 0.05, 0.1, and 0.3mm.

The Young’s modulus of the single α and β phase alloys are 17412 MPa and 79133MPa respectively, and Poisson’s ratio is 0.31. The measured parameters of stress and strain are used in FEM model shown in Table 2.
Fig. 3. 2D FEM model for the simulation (finer α grains)

Fig. 3 indicates the FEM model fine grain size of secondary phase (α). Two more FEM model are developed with different size i.e, medium and coarser grain sizes of secondary phase of Ti alloy (Fig. 4 and 5).

III. SIMULATION RESULTS

A. Comparison between the measured and simulated results of the Ti– alloy

By using the ANSYS software, the stress–strain curve of the 0.16α Ti– alloy was calculated based on the individual stress–strain curves of single-phase α and single-phase β, then compared with the measured results. The measured stress–strain curve and the simulated one by calculating with the two-dimension model are shown in Fig. 6. As there is little error between the measured result and the simulated one, but the curve fit is good. Therefore, the FEM used in this work is valid, which can be used for further simulation to analyze the effect factors and discussion for the distribution of micro-stress and strain of the 0.16α Ti–10V–4.5Fe–3Al.

The reasons for error between the measured curve and the simulated one are because of following assumptions.

1) Generally the microstructure is in three-dimensional form, but it is very difficult to build the 3D form hence the model is restricted to two-dimensional and this model adopted for simulation.

2) The regular elements are built by linking nodes, which is different from the real microstructure. The result will be also affected by the number of elements.

3) The shape and distribution of α phase in the model are not absolutely the same as the real one as well as its fraction; meanwhile, the errors can be caused by the inhomogeneous distributions in the microstructure.

4) The influence of grain boundary and interphase boundary is ignored in the model.

After the validation, the same FEM model used to for the simulation to know the effect of α grain size on the stress strain curve. After the simulation the stress strain curves are calculated at two different grain sizes and compared with the finer grain size. It is observed that the finer grain size curve is higher as compared with the other two coarser grain curves (Fig. 7).
Fig. 7. Comparison between the calculated stress-strain curves at different grain sizes of α (by kept volume percent of α is constant at 16%)

B. The analysis of the distribution of the stress and strain of the Ti–alloy

The stress distributions (First principle stress) are non uniform in all cases and also noted that the stress in the beta phase is higher than in alpha phase. Fig. 8 shows the stress distributions of Ti alloy at a displacement of 0.1mm for different grain sizes of secondary phase alpha. The maximum stress decreases with the increase of grain size, whereas the minimum stress increases with the increase of grain size of secondary phase α.

Fig. 8. First principle stress distributions at displacement of 0.1mm of Ti alloy at different grain sizes of α (at constant volume fraction α is 16%) (a) Finer (b) Medium & (c) coarser

Fig. 9. First principle elastic strain distributions at displacement of 0.1mm of Ti alloy at different grain sizes of α (at constant volume fraction α is 16%) (a) Finer (b) Medium & (c) coarser
Fig. 9. represents the first principle elastic strain distributions at 0.1mm of Ti alloy for different grain sizes of alpha phase. It is observed that the elastic strain is more in alpha phase as compared with the strain in the beta phase because the beta phase is harder than the alpha phase. It is also observed that the elastic strain increases with the increase in load.

Fig. 10. First principle plastic strain distributions at displacement of 0.1mm of Ti alloy at different grain sizes of alpha phase. It is observed that the plastic strain is more in alpha phase as compared with that of beta phase because the beta phase is harder than the alpha phase is softer. It is also observed that the plastic strain increases with the increase in load. The first principle total strain is the sum of plastic strain and elastic strain. The distributions of first principle total strain are similar to the distributions of first principle plastic strain. It also observed that the first principle total strain is more in alpha phase as compared to that of beta phase.

IV. CONCLUSIONS

1. The measured stress–strain curve of volume fractions of 0.16α is matches with the calculated curve, so the work is preferable and can be used for further simulation to analyze the effect of factors and discuss the distribution of micro-stress and strain of this alloy.

2. The distributions of first principle stress and strain in the α and β phases of the Ti-10V-4.5Fe-3Al alloy were simulated in all cases. The stress increases with an increase in the load, the maximum stress is in the β phase, whereas the minimum stress is in the α phase. The strain increases with an increase in the load too, whereas the maximum strain is in the α phase, and the minimum one in the β phase.

3. The stress strain curve of finer grain size is higher than the coarser one.

4. The maximum stress developed in the FEM model increases with the decrease in grain size of secondary phase i.e. α.

References