Numerical Simulation in relation to Adiabatic Shearing Behaviors in Titanium Alloy

Gao Ruihua1,2, Fan Qunbo1,2*, Wang Fuchi1,2

1 School of Materials Science and Engineering, Beijing Institute of Technology, 100081, Beijing, China, 2 National Key Laboratory of Science and Technology on Materials under Shock and Impact, Beijing, 100081, China

*Corresponding author e-mail: fanqunbo@bit.edu.cn

Abstract. The adiabatic shearing phenomena are commonly found in titanium alloys, but they are rarely simulated in the microstructure scale. In the current study, the macro-dynamic compression is implemented and the microstructures are successfully embedded into the macro model by introducing a multiscale simulation technique, thus help to reveal the adiabatic shearing deformation mechanism of titanium alloy. The simulation results show that for the equiaxed titanium alloy, the adiabatic shearing process is determined by the phase proportion outside the shear band instead of the phase proportion inside; the study further shows that within a certain proportion of α phase, with the increase of α phase proportion, the adiabatic shear sensitivity decreases.

1. Introduction

Titanium is an adiabatic shear-sensitive material, and it is easy to produce significant localized deformation under the condition of high strain rate and strain state, resulting in the formation of the adiabatic shear bands[1-3]. Adiabatic shear bands generated by thermal instability, when the effect of thermal softening predominates over the effect of strain hardening and strain rate hardening, give rise to plastic deformation instability into uniform plastic deformation localized deformation, forming of adiabatic shear band. The initiation of strain shear localization corresponding the highest point in the stress - strain curve, which indicates the loss of the carrying capacity of the titanium alloy materials, and the occurrence of plastic failure. The adiabatic shear deformation is an important aspect of the mechanical response of titanium alloy under high strain rate [4].

The adiabatic shear property of titanium alloy is closely related to its composition and microstructure. For the titanium alloys of the same composition, different microstructure morphology is associated with different adiabatic shear performances. On the titanium alloy of the relationship between the microstructure and the adiabatic shear performance, Zhang Wangfeng [5] adopted the linear regression method to study the impact of its anti-adiabatic shear properties of the titanium alloy sheet organization characteristic parameters, and obtained...
a function that could reflect the relationship between lamellar titanium anti-adiabatic shear properties, β grain size D, the α cluster size d, and α lamellar thickness b; based on Bayesian neural networks and fuzzy logic, S.K.Kar successfully implemented the prediction of the relationship between the microstructure characteristic parameters and the mechanical properties of the Ti-6Al-4V titanium alloy. However, these methods are not able to reveal the intrinsic mechanism of titanium alloy deformation process in the evolution of the microstructure, and the micro-level deformation information cannot be obtained. Therefore, it is particularly important to establish the relationship between microstructure and macro-dynamic compression, so as to study the effect of the characteristics on the titanium alloy adiabatic shear performance. In this paper, the LS-DYNA developed by Ansys and the microstructure oriented finite element software (MOF) developed by our group [6,7] are adopted to establish a multiscale simulation method for the titanium alloy adiabatic shear deformation, so as to study the key factor that dominates the adiabatic shearing sensitivity of equiaxed titanium alloy, and identify the influence of phase proportion on adiabatic shear sensitivity.

2. Multiscale simulation of titanium alloy adiabatic shear deformation

In the current study, the multiscale simulation method of titanium alloy adiabatic shear deformation is proposed by establishing the macro finite element model first, extracting the boundary conditions from a specified micro region subsequently, exerting the boundary conditions on the finite element model of the microstructure, finally calculating with LS-DYNA.

2.1. Macro-dynamic compression

The macro-dynamic compression finite element model is shown in Figure 1. The specimen is a 2D axisymmetric finite element model, subdivided by 2000 elements, and element size is set to 25μm. As shown in Figure 1, the radius and the height are 5mm, respectively. The upper edge is applied by a rigid wall, the lower edge is constrained in the vertical direction, and the friction coefficient between the upper edge and the rigid wall is 0.08. In order to ensure the strain rate of approximately 3400/s, the rigid wall is loaded by the speed of 17m/s, and the time of macro-dynamic compression is 80μs. Since large local shearing deformation will happen along the 45° diagonal direction for a macro-dynamic compression sample, serious element distortion will happen if with the traditional Lagrange algorithm. Therefore, the Arbitrary-Lagrangian-Eulerian algorithm (ALE algorithm) is adopted in this current study [8], which optimizes those distorted elements accordingly, thus keeping the calculation stability.
2.2. The numerical simulation of adiabatic shear deformation for titanium alloy

The numerical simulation of adiabatic shear deformation for titanium alloy is shown in Figure 2. Firstly, a 300μm × 300μm micro region to be studied is selected from the macrostructure finite element model, while the model is fully discretized in order to accurately track the nodal displacements history data within this region; then, finite element mesh generation principle combined with digital image processing approach has been used to generate the equiaxed finite element model based on the actual microstructural images. In this paper, the model is subdivided by 40000 elements, and element size is set to 1.5μm. While the micro model is loaded by the boundary conditions that extracted from the macro mode, and a secondary analysis calculation is carried out, in order to achieve the deformation information inside the micro region on a smaller scale.

Figure 1. Titanium alloy macro-dynamic compression finite element model

Figure 2. The numerical simulation of adiabatic shear deformation for titanium alloy
3. The influence of equiaxed microscopic characteristics on titanium alloy adiabatic shear sensitivity

Adiabatic shear sensitivity of titanium alloy is closely related to many factors, such as the phase proportion, phase size, and phase morphology. In this current study, however, the phase proportion is focused on. The phase proportion contains the phase proportion inside the adiabatic shear band, and the phase proportion outside adiabatic shear band. These factors influence each other, thus it is difficult to determine which one is the key factor. Meanwhile, the strength of β phase is stronger than α phase, and the α phase has a better uniform plastic deformation ability than the β phase has. Therefore, these issues will be focused on.

3.1. The influence of the phase proportion within the shear band on adiabatic shear sensitivity of equiaxed titanium alloy

Because plastic deformation is mainly concentrated in a narrow adiabatic shear band in the process of adiabatic shearing deformation, it seems that the phase proportion within the shear band dominates the adiabatic shear sensitivity. Therefore, the effect of the α phase proportion within the adiabatic shear band on the adiabatic shear sensitivity is discussed firstly. Three equiaxed titanium alloys with different microstructure characteristics are designed, as is shown in Figure 3 (a)–(c), where the blue is α phase, the red is β phase. Based on the micro model, the contours of strain are achieved by further calculation, as is seen in Figure 3 (d)–(f). The statistics show that α phase proportions within the shear bands are 60.6%, 22.5%, 14.3%, respectively.

![Figure 3. The equiaxed titanium alloys with different α phase proportions within shear bands](image)

(a) (d), 14.3%; (b) (e), 22.5%; (c) (f), 60.6%

The calculation method of Section 2.2 is adopted to calculate crack initiation time, and the result is shown in Table 1. As is seen in Table 1, little change is found when the α phase proportion within the shear band is varied from 60.6% to 14.3%, and the maximum difference is only 0.8μs, which indicates that the phase proportion
within the shear band has little influence on adiabatic shear sensitivity for equiaxed titanium alloys. Therefore, it is not the key factor that dominates the adiabatic shear sensitivity.

**Table 1.** The crack initiation time of equiaxed titanium alloys with different α phase proportions within the shear bands

| α phase proportion (%) | Crack initiation time (μs) |
|------------------------|---------------------------|
| 14.3                   | 42.5                      |
| 22.5                   | 43.3                      |
| 60.6                   | 42.7                      |

3.2. The influence of the α phase proportion outside the shear band on adiabatic shear sensitivity of equiaxed titanium alloy

In the present work, a series of equiaxed titanium alloys with different microstructure characteristics are constructed. The α phase proportion distributed in the direction of 45° is kept constant, while the α phase proportion outside the shear band is continuously changed. As is shown in Figure 4 (a)–(f), the α phase proportions outside the shear bands of equiaxed titanium alloys are 13.8%, 20%, 27%, 34.7%, 42%, 46%, respectively.

**Figure 4.** The equiaxed titanium alloys with different α phase proportions outside the shear bands

(a) 13.8%; (b) 20%; (c) 27%; (d) 34.7%; (e) 42%; (f) 46%

As is shown in Figure 5, when the calculation time is 44μs, the strain contours corresponding with different α phase proportion are presented accordingly.
Figure 5. The effective plastic strain contours with the calculation time is 44μs

(a) 13.8%; (b) 20%; (c) 27%; (d) 34.7%; (e) 42%; (f) 46%

As is seen in Figure 5, the strain localization region is readily observed in the direction of 45°, leading to the formation of the adiabatic shear band. When the α phase proportion outside the shear band is varied from 13.8%~46%, with the increase of the α phase proportion, the strain localization region decreases. For the α phase proportion of 13.8%, it has the largest strain localization region, the highest strain is more than 2.9, and the initiation of apparent cracks are observed; however, when the α phase proportion increases to 46%, the highest strain is lower than 0.7, and the strain localization region almost disappears. In order to further study the phenomenon, influence of the α phase proportion outside the shear band on adiabatic shear sensitivity is calculated and shown in Figure 6. The results show that as the α phase proportion changes from 13.8% to 46%, the crack initiation time is varied from 40.1μs to 46.2μs, and the difference of crack initiation time is up to 6.1μs, which indicates the α phase proportion outside the shear band is the key factor that dominates the adiabatic shear sensitivity of equiaxed titanium alloys and the adiabatic shear sensitivity decreases with increasing α phase proportion within a certain proportion of α phase. The research further shows that since the α phase has a better uniform plastic deformation ability than the β phase has, with the increase of the α phase proportion, the uniform plastic deformation ability increases, resulting in a decreased tendency of strain localization, thus the adiabatic shear sensitivity decreases[9-11].
Figure 6. The crack initiation time of equiaxed titanium alloys with different $\alpha$ phase proportion

4. Conclusions
In the current research, the macro-dynamic compression is implemented and the microstructures are successfully embedded into the macro model by introducing a multiscale simulation technique, so as to study the influence of the phase proportion on the adiabatic shear sensitivity of equiaxed titanium alloy. The main conclusions are as follows:

(1) The phase proportion within the shear band has little effect on the adiabatic shear sensitivity of equiaxed titanium alloy.

(2) For the equiaxed titanium alloy, the phase proportion outside the shear band is the key factor that dominates the adiabatic shear sensitivity.

(3) Within a certain proportion of $\alpha$ phase, with the increase of the $\alpha$ phase proportion outside the shear band, the adiabatic shear sensitivity decreases.

5. Reference
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