Finite element simulations on the relation of microstructural characteristics and the formation of different types of adiabatic shear bands in a β-titanium alloy

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Abstract. Deformation at high strain rates in combination with local thermal softening can lead to the formation of so-called adiabatic shear bands. These shear bands occur when the macroscopic deformation is concentrated in microscopic areas. The fundamental thermomechanical processes and micromechanical mechanisms acting during adiabatic shear band formation are not fully understood yet. In particular, the influence of different initial microstructures on shear band formation has not sufficiently clarified. In an earlier investigation, adiabatic shear bands formed in a β-titanium alloy with different initial microstructures were characterized in detail. It was shown that different volume fractions of the α-phase result in the formation of different types of shear bands. In the present study, a simple modeling approach based on the finite element (FE) method is used to investigate in a systematic parameter study (with a special focus on mechanical and thermal variables) how these different types of adiabatic shear bands can occur in the same material. The FE simulations clearly show that microstructural characteristics – such as size and volume fraction of the α-phase in the β-titanium alloy – have a strong influence on shear band formation. This study contributes to a more detailed understanding of the microstructural and thermomechanical mechanisms leading to the formation of different types of adiabatic shear bands in titanium alloys.

1. Introduction and experimental background

Because of their low thermal conductivity, titanium alloys are susceptible to the formation of adiabatic shear bands (ASB) [1–3]. Generally, ASB occur at high strain rates (\(<10^2\) s\(^{-1}\)) when the macroscopic deformation is concentrated in microscopic areas [4,5]. This leads to a local temperature increase because the heat cannot be dissipated quickly enough into the surrounding material. This effect results in local thermal softening which in turns leads to a further concentration of deformation in this region of the sample.

The mechanical behavior of β-titanium alloys is strongly affected by microstructural parameters like β-grain size, morphology and volume fraction of primary and secondary α-phase precipitates [6–9], but the effect of these microstructural features on shear band morphology is not yet well understood. The present study is part of an ongoing experimental and theoretical investigation on the evolution of adiabatic shear bands in the β-titanium alloy Ti-10V-2Fe-3Al for different types of initial microstructures: β-titanium with primary α-phase and β-titanium with primary and secondary α-phase
precipitates. We carried out extensive compression-shear tests in a previous experimental study [10] to specifically characterize the influence of the different initial microstructural characteristics on the formation of ASB. Compression-shear specimens, proposed by Meyer et al. [11], are geometrically derived from conventional cylindrical compression samples, but the top and lower surfaces are cut at a small angle of inclination with respect to the central axis. When loaded in compression, this special geometry leads to a superposition of shear stresses. While the resulting stress state is inhomogeneous [12], compression-shear specimens allow to test a material for its tendency to exhibit localized (shear) deformation. Compression-shear testing has been successfully used to characterize localized deformation in functional materials [13,14], where complex stress-states can considerably affect phase transitions [15]; this technique is, moreover, specifically well-suited to analyze the formation of ASB and subsequent material failure in structural materials at high strain rates [16,17]. All experiments considered here [10] were performed on compression-shear specimens (width a height and width of 6 mm and an angle of inclination of 6°) in a Split-Hopkinson pressure bar (initial strain rate: $10^3 \text{ s}^{-1}$), [18,19]. Deformation was stopped at a nominal (uniaxial) compressive strain of 10 % for each microstructural condition, facilitating an investigation of the different stages of nucleation and propagation of the shear bands. Our results confirmed that the formation mechanisms of adiabatic shear bands strongly depend on the initial microstructure [20]. Two different types of adiabatic shear bands can occur in the deformed compression-shear specimens, as exemplarily shown in Figure 1.

![Figure 1. Scanning electron micrographs of two differently heat-treated states of the β-titanium alloy Ti-10V-2Fe-3Al, after 10 % nominal axial deformation of a compression-shear specimen (strain rate $10^3 \text{ s}^{-1}$). a) The single-step heat-treated state $A(\alpha_p)$ exhibits the primary α-phase (dark zones) with a volume fraction of about 40 %. This state forms a single adiabatic shear band (ASB) with a width of 5 µm. b) The two-step heat-treated state $A(\alpha_{p+s})$ contains the same content of primary α-phase and an additional volume fraction of about 15 % of the secondary α-phase. This state forms ASBs that are characterized by many fine branches.](image)

Figure 1a) shows a typical ASB in the single-step heat-treated state $A(\alpha_p)$, which was aged at a temperature of 700 °C for 1h. This state exhibits about 40 vol.-% of the lamellar primary α-phase ($\alpha_p$), which is precipitated according to the Burgers relationship [21]. When shear deformation occurs, a major part of the plastic deformation is transmitted to the lamellar α-precipitates (black lamellar structures in the scanning electron microscopy (SEM) images). In addition, a rotation of the α-precipitates towards the propagation direction of the adiabatic shear band is observed. Inside the shear band, there is a strong deformation of the α-precipitates in the shearing direction. The thick shear band completely deforms a volume width a characteristic thickness of about 5 µm. Figure 1b) shows a similar micrograph of the material heat-treated in two steps (step 1: similar to the condition $A(\alpha_p)$; step 2: additional aging at 500 °C for 8h). This material condition differs from $A(\alpha_p)$ only by an additional volume fraction (about 15 %) of the secondary α-phase ($\alpha_s$), which is also precipitated according to the
Burgers relationship. The content and size of the primary $\alpha$-phase are very similar to the one-step heat-treated condition. Moreover, the macroscopic stress-strain behavior of the two material conditions is also very similar [20]. Interestingly, however, the stopped compression-shear experiments demonstrate that the secondary $\alpha$-phase content leads to the formation of a quite different, branching type of ASB [20]. The additional lattice strain in the material, introduced by the smaller secondary $\alpha$-phase precipitates, prevents rotation of the large primary $\alpha$-precipitates during shearing. It is assumed that, due to the smaller distances between the different $\alpha$-precipitates, the shear band is deflected by the very small $\alpha_s$-precipitates (average size below 200 nm, [20]) when passing through the $\beta$-matrix. Because of the lower strength of the $\alpha$-phase [22] the shear band propagates predominantly along an $\alpha$-rich path.

The stopped compression-shear experiments and in particular the subsequent microstructural investigations of the specimens [20] summarized briefly above have clearly shown that an increased volume fraction of the $\alpha$-phase (by means of finely precipitating secondary $\alpha$-phase) strongly influences the evolution of ASB - in particular in the nominal deformation range of 10 $\%$, where the shear bands still propagate in the compression-shear specimens and the material has not yet failed. The present study is motivated by these experimental findings and aims at identifying microstructural parameters that affect the formation and propagation of the different types of ASB by simple numerical simulations. We present first results obtained from a simple Finite Element (FE) modeling approach, considering a model system that shows how different types of ASB can be formed in the same base material, but with different initial microstructures. The systematic parameter study identifies simple but relevant relations between mechanical, microstructural and thermal parameters and ASB propagation.

2. Finite element simulations

For this study, 2D FE simulations were performed with the commercial FE package *Abaqus*. Because of the strong effects of both strain rate and temperature on ASB formation, the FE simulation was mechanically-thermally coupled and dynamically explicit calculations were performed. A 2D compression-shear specimen was modeled with an inclination angle of 6° similar to the geometry of the samples used in our previous experiments (Figure 1). The inclination of the sample is necessary to locally create shear stresses that can result in shear localization during loading. For the numerical compression-shear tests, various (much simplified, but based on the real microstructure of the single-step heat-treated $A(\alpha_p)$ state) microstructures were modeled. In the simulations, the microstructure had to be represented by two different material definitions. The matrix approximated the behavior of $\beta$-titanium and the precipitates that of $\alpha$-titanium.

The parameters used in the simulations are summarized in Table 1. To model the $\alpha$-phase, material parameters of pure $\alpha$-titanium from literature [23] were assumed for the modulus of elasticity, density, thermal conductivity and specific heat capacity. The parameters for $\beta$-titanium correspond to experimentally determined values of the solution-annealed condition of the alloy Ti-10V-2Fe-3Al [24]. To model the elasto-plastic behavior, a flow curve of the state $A(\alpha_p)$ (determined experimentally in a compression test under quasi-static conditions, [20]) was used for the $\beta$-titanium matrix. This state represents the macroscopic mechanical behavior of a hardened matrix with lamellar $\alpha$-precipitates the most. According to [22], the $\alpha$-phase has a lower strength than the surrounding $\beta$-titanium microstructure; therefore the flow curve of the matrix was multiplied by 0.5 in a first order approximation to account for the properties of the $\alpha$-precipitates (Figure 2). This corresponds to the strength of pure grade 3 $\alpha$-titanium [25] and can be considered as a realistic value for the material definition.

The area below the flow curves corresponds to the energy introduced into the material in the simulated compression-shear test. The Taylor-Quinney factor, determining the fraction of the total energy that is converted to heat and thus increases the temperature in the material [26], was assumed to be 0.9 for the entire simulation, which is a common value for the simulation of ASB [27–29], although recent work [30] shows that the Taylor-Quinney factor can be strongly material-dependent.
While both thermal softening and the strain-rate dependence of the material (which strongly affect ASB formation in a macroscopic mechanical test) were not considered in our simulations, the boundary conditions and the special geometry of the 2D sample ensured that localized deformation occurred. While highly simplified, our simulations therefore still allowed to qualitatively analyze the effect of different microstructural parameters on ASB formation.

**Table 1.** Parameters for the material definitions of the $\beta$-titanium matrix and the $\alpha$-titanium precipitates.

|                      | $\alpha$-titanium – Ti($\alpha$) (precipitates) | $\beta$-titanium – Ti($\beta$) (matrix) |
|----------------------|------------------------------------------------|------------------------------------------|
| Young's modulus in MPa | 105000                                          | 110000                                   |
| Poisson's ratio       | 0.3                                             |                                          |
| flow curve            | $\text{Ti}(\alpha) = 0.5 \cdot \text{Ti}(\beta)$ | $\text{Ti}(\beta) = [\text{flow curve } A(\alpha_p)]$ |
| density in $\text{g/cm}^3$ | 4.5                                              | 4.6                                      |
| thermal conductivity in $\text{W/m}\cdot\text{K}$ | 22                                               | 8                                        |
| specific heat capacity in $\text{J/Kg}\cdot\text{K}$ | 523                                              | 560                                      |
| Taylor-Quinney factor | 0.9                                              |                                          |

**Figure 2.** Flow curves of the matrix ($\text{Ti}(\beta)$) and the precipitates ($\text{Ti}(\alpha)$) that were used for the FE simulations. The flow curve for $\text{Ti}(\beta)$ was determined experimentally under quasi-static conditions (state $A(\alpha_p)$) in a conventional compression test. The flow curve of the softer $\alpha$-phase was approximated by multiplication of the curve of $\text{Ti}(\beta)$ by 0.5.

The mesh of the compression shear sample consisted of 4-node elements (CPE4RT); the mesh at the precipitates was finer than that in the adjacent sample volume. In a sample with, for instance, 90 precipitates, we used approx. 14300 elements. We did not include grain boundaries, i.e., the simulated sample in a first approximation represents a single grain in which localized shear occurs due to the geometric/mechanical instability. To reduce computation times for this first parameter study, a plane-strain state was assumed, and friction effects (e.g., between the sample and an experimental setup) were neglected. The specimen was instead deformed by simply applying a strain rate of $10^3 \text{ s}^{-1}$ directly at the top and bottom (displacement boundary conditions). Below, the simulation results are presented at 10 % nominal plastic deformation, to allow for a qualitative comparison with the experimental results from our previous studies.
3. Results and discussion

Figure 3 shows results of the modeled compression-shear test in terms of the undeformed specimen (labeled “structure” in Figure 3) the distributions of equivalent (von Mises) stresses and strains, respectively. In order to be able to represent an initial condition as a reference configuration, a specimen consisting only of pure β-titanium structure (without precipitates) is considered first. The calculated stress distribution at 10 % nominal axial compression shows the expected stress concentration along the short diagonal of the specimen. The deformation is therefore also concentrated almost entirely in a small band along the shortest diagonal. We do not analyze the deformation of the sample near its corners in detail because it is primarily related to the simplified (displacement) boundary conditions used in the present study. The calculated strain in the shear plane is significantly higher at the corners than in the middle of the specimen; this agrees well with more realistic simulations of the three-dimensional compression-shear samples, [12]. The specimen shape used for the simulation is therefore well suited to produce a stress concentration together with a strongly localized deformation in a narrow area, which can be observed in the calculated stress and strain fields. Deformation of the precipitation-free matrix material (used as a simple reference condition) leads to a closed structure of the shear band.

In the following, the influence of microstructural parameters on shear band formation is examined in greater detail. For this purpose, different amounts of precipitates (approximated to have an oval shape) with the material definition of α-titanium were added to the β-titanium matrix. The precipitates represent the lamellar primary α-phase and are thus oriented similar to the (2D) Burgers relationship: the angle between individual precipitates is always 60°, resulting in three different orientations. To define a regular distribution of these precipitates, the first precipitate was oriented with an angle of 0° and placed in the lower left corner of the compression-shear sample. The next one was moved at a defined distance (depending on the total number of precipitates to be considered in the different simulations) in X-direction and rotated by 60°. This process was repeated (in X- and Y-direction, using further rotations by 60°) until the sample was filled with a regular pattern of precipitates.

Figure 4 (presenting information in a layout similar to Figure 3) shows three microstructures with different amounts of precipitates (the labels in the top row correspond to the number of precipitates in X-direction multiplied by the number in Y-direction) and the corresponding stress and strain fields. Changing the number of precipitates (and, to preserve the volume fraction of the α-phase, changing their size) clearly affects shear band formation. In the 5 x 4 sample with relatively large precipitates, the calculated stress field shows that there is not a single monotonous stress concentration (as in the pure β-microstructure): Instead, in the shear plane between the precipitates, areas with significantly lower equivalent stress values are observed. This is directly related to the lower strength of the
precipitates that consequently carry much of the deformation (and thus partially unload the surrounding matrix). The strain field shows a deflection of the main region of deformation out of the shear plane; a slight splitting into two shear bands can be observed, where the deformation is primarily localized on an α-phase rich path in (and in proximity to) the shear plane. The deformation is somewhat more pronounced in the upper shear band, which is most likely related to the location and orientation of the precipitates next to the upper left corner.

Figure 4. Simulated microstructures and the corresponding stress and strain fields at 10 % axial compression for different sizes of α-precipitates (at a constant volume fraction of 17.5 %). With increasing number of (soft) precipitates in the shear plane, the tendency to deflect or split the shear bands increases significantly.

When the number of precipitates is increased to 90 (10 x 9) or 210 (15 x 14), the calculated strain fields show a more pronounced tendency for shear band splitting. As more (and finer) precipitates lie in or directly next to the shear plane, growth of the initial shear band is more strongly affected by the α-phase, and individual precipitates can deflect the growth direction of the shear band by offering a path of low resistance to mechanical deformation. Because of the presence of many smaller α-lamellae, shear band splitting can occur more easily. Depending on the orientation of the particles, either a deflection or splitting of the shear bands occurs at different points in the simulated samples. This leads to the formation several approximately parallel shear bands and a more widely spread region of increased stresses compared to the pure β-titanium reference simulation. To summarize, the presence of the α-phase, and the sizes, orientation and distribution of the corresponding precipitates,
clearly affect shear band formation. Despite the many simplifications used in our 2D simulations, this behavior agrees well with the experimental observations on shear band formation in the two aged states (Figure 1). The state \( A(\alpha_{p+s}) \) is characterized by a significantly higher amount of small \( \alpha \)-precipitates and also tends quite strongly to deform by the formation of branched ASB.

![Figure 5](image_url)

**Figure 5.** Simulations of representative microstructures with different volume fractions (but constant particle size) of the \( \alpha \)-phase at 10 % axial compression. A certain critical volume fraction of precipitates in the microstructure (17.5 %) is necessary in order to observe shear band branching into two sub-bands running parallel to the shear plane. If the content (and thus also the particle spacing) is too low (10 %), a closed band is formed that passes primarily through the \( \beta \)-matrix. If particle distances are too short and/or the volume fraction is high (25 %), deformation is redistributed into the soft \( \alpha \)-lamellae.

The simulation results presented in Figure 5 show the influence of different volume fractions (at a constant particle size) of the \( \alpha \)-precipitates on ASB formation. The compression-shear test with a volume fraction of 17.5 % corresponds to the previous 10 x 9 sample (Figure 4). As already discussed, this condition is characterized by a deformation in two shear bands that are formed parallel to the shear plane. When the volume fraction is reduced to 10 %, the mean distance between the precipitates is obviously too large for deflection or branching of the shear band. Only one main shear band is formed, which runs predominantly through the \( \beta \)-matrix. Only in areas where the precipitates are aligned perpendicular to (and across) the shear plane, the deformation partially occurs in the precipitates. Interestingly, when the volume fraction is instead increased to 25 %, there is also no
distinct branching of the shear band (as observed in the corresponding strain field plot). Due to the significantly lower strength of the precipitates, most of the deformation in the shear plane can occur in the closely packed precipitates. The main path for the propagating shear band then is located inside the α-lamellae, which are positioned conveniently and in sufficient number in the main shear plane of the sample. Because the distance between the precipitates is small, strain is concentrated in the closely spaced softer precipitates and can also be deflected orthogonally (even away from the shear plane, but only inside additional precipitates). Clearly, this very high content of the α-phase leads to a widely spread strain field into the proximity of the shear plane even though branching of the ASB cannot be observed.

In summary, the simulation results show that shear band splitting and deflection is directly affected by the volume fraction of α-precipitates. When the volume fraction is too low, deformation occurs primarily in the β-matrix in a closed shear band. When, in contrast, the volume fraction is too high (and hence the distances between precipitates are very small), the energy introduced into the sample during deformation is consumed and distributed mainly into the softer precipitates. Consequently, there is no well-defined, localized deformation in the shear plane. Considering real microstructures as observed in [20], this means that a critical volume fraction of α-phase must be present in β-titanium in order for ASB to form distinct branches. In our simple and qualitative 2D FE simulations, the critical volume fraction is approx. 17.5% in the 10 x 9 compression shear specimens. In the actual experiments, ASB branching was observed in the state A(α_{p+s}) with approx. 55% α-phase (α_p + α_s), whereas in the material state A(α) (with approx. 40% α_{p}-phase and larger distances between the individual lamellae) only a homogeneous shear band occurred, which corresponds closely to the simulated sample 10 x 9 with 10% of the α-phase.

4. Summary and conclusions

In the Ti-10V-2Fe-3Al material conditions tested experimentally in our previous studies, the formation and propagation of ASB is characterized by the complex interaction of, for example, microstructure, temperature, multi-axial stress states (as well as local stress gradients), physical properties of matrix and precipitates, and strain rate. While the 2D FE simulations performed in the present study cannot, as expected, provide quantitative information on critical microstructural parameters for ASB type selection, the simple model system investigated numerically does allow for an evaluation of relevant microstructural trends that are in good agreement with our experimental observations. Particularly the information on a critical volume fraction of the α-phase, and on the effect of soft phases providing favorable pathways for shear band growth, provides a basis for further investigations into the interesting phenomenon of ASB branching in Ti-10V-2Fe-3Al.

In summary, the following main results on the influence of microstructure on shear band formation in Ti-10V-2Fe-3Al can be directly applied to qualitatively interpret experimental observations:

1) The tendency to split a shear band increases significantly with increasing number and decreasing size of soft α-lamellae in the shear plane.

2) A critical volume fractions of the α-phase in the β-titanium matrix must be reached before branching of shear bands can occur.

3) Increasing free distances between α-precipitates, in contrast, lead to the formation of conventional shear bands without branching.

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