Mechanical behavior and texture prediction of Ti-6Al-4V based on elastic viscoplastic self-consistent modelling

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Abstract. The goal of this study is to apply an elastic viscoplastic self-consistent crystal plasticity model to predict the texture evolution in a Ti-6Al-4V alloy which has a (mainly) hexagonal crystal structure. The model under consideration is an extension of the viscoplastic self-consistent model proposed by Lebensohn and Tome [1993] which has been adapted to account for elasticity and has been integrated with a new algorithm, making it more computationally efficient within an implicit FE scheme. The flow behavior of Ti-6Al-4V is strongly dependent on strain rate and temperature. To estimate the model parameters, the flow behavior of quasi-static experiments is used. A temperature sensitivity term has been introduced to correct the effects of temperature increase during the dynamic experiments. In order to have a meaningful rate sensitivity exponent, a value is calculated based on valid experimental data, rather than choosing an arbitrary large numerical value. In this way the behavior of Ti-6Al-4V is captured at different strain rates. Predictions of the model are compared to experimental data.

1. Introduction

Polycrystal models are a family of constitutive models that can be used both as a constitutive model and a tool for performing virtual experiments for other constitutive models. VPSC and ALAMEL are examples of polycrystal models, which have been successfully used for texture and anisotropy estimation of HCP metals [1, 2].

Ti-6Al-4V accounts for more than 50% of total titanium usage thanks to its bio-compatibility, high strength-to-weight ratio and good corrosion resistance [3]. HCP titanium alloy exhibits four slip systems: basal {0 0 0 1} <1 1 2 0>, prismatic {1 0 1 0} <1 1 2 0>, first order pyramidal {1 0 1 1} <1 1 2 0>, and second order pyramidal {1 0 1 1} <1 1 2 3>. Plastic deformation is mostly accommodated by basal or prismatic slip along burgers vector <a>, whereas slip is more difficult on the pyramidal slip systems. Besides slip, twinning can be also active in tensile {1 0 1 2} <1 0 1 1> or compressive {1 1 2 2} <1 1 2 3> mode. To accommodate strain parallel to the c axis of the hexagon, second order pyramidal or twin systems should be activated [4]. Although pure titanium is known to exhibit extensive primary and secondary twinning, the high amount of aluminum in Ti-6Al-4V prohibits formation of extensive twins. In monotonic modes of deformation at room temperature, only very low volume fractions (less than 1%) of tension twins have been observed. According to Hammami et al. [2] and Jones and Hutchinson [5] cross-slip occurs along the <c+a> vector on pyramidal planes during uniaxial compression, while it is absent during uniaxial tension.

In this work, the parameters needed for the VPSC90 model [6] (updated version of VPSC) are derived using standard tensile tests at different quasi-static strain rates and an improved fitting procedure, which involves VPSC90. Subsequently, these parameters are used to predict the mechanical behavior and texture development in during quasi-static and dynamic loading.
2. Experimental setup

2.1. Material

The Ti-6Al-4V sheet has a thickness of 0.6 mm. The mill-annealed condition results in equiaxed $\alpha$-phase grains (96% vol. fraction and average grain size of 6 $\mu$m) and bcc $\beta$-grains (4% vol, average grain size of less than 1 $\mu$m).

![Microstructure of sheet in RD-ND plane for $\alpha$ and $\beta$-phases, respectively, b) {0001} pole-figure of the $\alpha$-phase, which shows the orthorhombic sample symmetry.]

Because of its low volume fraction, the $\beta$ phase is neglected in the model. The $\alpha$-phase texture is shown in figure 1-b, which clearly shows a typical hexagonal texture. Two symmetric components along the ND-RD plane with basal poles oriented in the TD direction can be seen, which are attributed to remaining effects of the hot rolling process. Two other symmetric components along ND-TD plane with deviation from the ND pole towards RD are also noticeable. The latter components are attributed to the residual effects of cold rolling.

2.2. Mechanical Testing

Quasi-static and dynamic tension experiments were performed. Samples were cut along the rolling direction of the sheet. Quasi-static experiments at moderate strain rates were used to fit the model parameters. To guarantee the quasi-static conditions and to obtain isothermal flow curves, thermal effects of strain rates were taken into account using a thermo-mechanical model [7]. Dynamic tests were performed using the Split Hopkinson Tensile Bar (SHTB) method. Subsequently, using the parameters obtained from quasi-static tests, the mechanical behavior of the material at high strain rates was investigated.

3. Modelling

Since the effects of temperature and strain rate can be separated, the parameters obtained by fitting the mechanical behavior at quasi-static conditions should be able to describe the material behavior both at quasi-static and dynamic loading situations. Non-isothermal flow curves of quasi-static experiments ($8\times10^{-5}, 6.7\times10^{-4} \text{s}^{-1}, 5\times10^{-2} \text{ and } 5\times10^{-1} \text{s}^{-1}$) were transformed to isothermal curves using a thermomechanical model based on the Johnson-Cook hardening model [7]. The different slip systems of $\alpha$ titanium considered here are prismatic, basal, pyramidal $<a>$ and pyramidal $<c+a>$. Since the twinning fraction observed both in literature and in this work for tensile deformation is very low, twinning systems were excluded from the model. The ODF of the initial material, derived from the orientation contrast scans, is discretized in 1000 orientations for the purpose of the simulation. Voce hardening parameters obtained by fitting are shown in table 2.
Table 2: Voce hardening parameters for α titanium; Latent hardening for all slip systems is equal to 1.

| Deformation mode | ν₀   | τₛ₀   | τₛ₁   | Θₛ₀ | Θₛ₁ |
|------------------|------|-------|-------|-----|-----|
| Prismatic        | 88   | 390   | ---   | 0   | 0   |
| Basal            | 81   | 427   | 46    | 170 | 0   |
| Pyramidal <a>    | 124  | 457   | 852   | 350 | 0   |
| Pyramidal <c+a>  | 76   | 549   | 657   | 1040| 0   |

The simulated tensile curves shown in figure 2 are the results of the fitting procedure. From this figure it is clear that an excellent agreement is obtained between the simulated and experimental curves: the model reproduces both the hardening behavior and the strain rate sensitivity.

![Figure 2: comparison of experimental (black points) and simulated (colour lines) tensile curves.](image)

To assess the capability of the model to predict the mechanical behavior, post-necking local strain measurements obtained by high speed imaging and a DIC technique for a quasi-static (6.7×10⁻⁴ s⁻¹) and a dynamic test (average 425 s⁻¹) were investigated.

![Figure 3: simulated flow behavior for 0.00067s⁻¹ and 425s⁻¹ together with the corresponding slip system activity.](image)

4. Results and discussion

The simulation results of the tensile experiments, together with the slip systems activities, are shown in figure 3. The hardening behavior is very well reproduced. Even though the tensile curve obtained by dynamic behavior displays some oscillations, and the strain rate is not constant during the experiment, a good agreement is obtained. The slip systems activity diagrams show that most of the deformation is accommodated by prismatic slip, followed by the basal slip, while the two pyramidal slip systems have minor activity, which even further
decreases at higher strains. Although activation of pyramidal $<c+a>$ is more difficult than pyramidal $<a>$, its contribution to deformation is higher, thus compensating for deformation in the $<c>$ direction of the hexagonal unit cell. No considerable amount of twinning was observed by EBSD inspection both for quasi-static and dynamic cases, and the right prediction of hardening behavior by only considering dislocation glide is thus confirmed. An EBSD measurement of the material adjacent to the fracture zone of a quasi-static tensile sample ($6.7 \times 10^{-4} \text{s}^{-1}$) with almost 30% deformation, together with the simulated texture prediction is represented, cf. figure 4. In the experimental pole figure (Fig. 4a), weakening of the initial rolled components is observed, while new components develop which exhibit the basal plane normal parallel to the rolling direction. The simulated texture (Fig. 4b) shows that without considering twinning the most important features of the experimental texture can be reproduced.

The results represented here show that the VPSC model can be successfully applied for constitutive modelling of Ti-6Al-4V. It is of relevant importance to observe that in spite of all the simplifications, such as considering only one phase and only 1000 grains, the mechanical behavior can still be captured for a wide range of strain rates. Although texture changes are more severe in large deformation processes and in the presence of compressive forces, still the VPSC polycrystal model is capable of tracking texture changes.

![Figure 4](image-url)

Figure 4: texture evolution in quasi-static deformation at $6.7 \times 10^{-4} \text{s}^{-1}$ after 30% deformation. (a) The experimental pole figure and (b) the simulated one.

5. Conclusion

Quasi-static and dynamic tensile tests were conducted on Ti-6Al-4V. Using the quasi-static data and taking into account the initial texture, the VPSC model parameters were determined by a series of tensile tests. These parameters were successfully applied to simulate the large deformation behavior of material at quasi-static and dynamic cases. No considerable amount of twinning was observed; both texture prediction and hardening behavior of the material are supporting this idea.

Acknowledgments

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References

[1] Lebensohn R A and Tomé C N, 1993, Acta Metall Mater, 41, 2611-2624.
[2] Hammami W, Gilles G, Habraken A M, Duchene L, 2011, Int J Mat Form, 2, 205-215.
[3] Bedinger G M, Titanium Minerals Yearbook, 2013, United States Geological Survey.
[4] Cazacu O, Plunkett B, Barlat F, 2006, International Journal of Plasticity, 7, 1171-1194.
[5] Jones I, Hutchinson W, 1981, Acta Metallurgica, 6, 951-968.
[6] Galán J, Verleysen P, Lebensohn R A, 2014, Modelling Simul. Mater. Sci. Eng, 22, 5, 055023
[7] Galán J, Verleysen P, Degrieck J, 2013, Strain, 49, 4, 354-365.