

MULTISCALE FINITE ELEMENT STUDY OF TI-555

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ABSTRACT The material parameters of the 2 phases Ti-555 alloy have to be extracted in order to perform simulations on representative microscopic cells and guide the optimization of the alloy. The identification of the flow parameters of the BCC β -phase is discussed, using macroscopic and microscopic constitutive laws. The validation is performed, comparing experimental and numerical tensile tests obtained for different strain rates.

INTRODUCTION: Ti-555 is a new generation of Ti alloy that should be suitable for aeronautical applications. Generally, it is composed of a BCC β -phase and a hexagonal α -phase. Numerical simulations are performed to optimize its microstructure and then to guide the thermal treatments imposed to the material. The Finite Element Code Lagamine developed at the University of Liege is used here and two constitutive laws are chosen to model the behavior of the β -phase of Ti-555 at different strain rates. The experimental tests are firstly presented. Then, the macroscopic Norton-Hoff and the microscopic elasto-viscoplastic crystal plasticity-based constitutive laws are briefly described. The results obtained with both laws are finally presented and discussed.

PROCEDURES, RESULTS AND DISCUSSION:

Experimental Tests: Experimental tensile tests were performed at different strain rates on 100 % β Ti-555 material (Fig.1.).

Numerical Constitutive Laws: In this study two constitutive laws are used. The first one is a Norton-Hoff law modified to introduce softening. The following formulation was proposed by [Pascon *et al.* 2007]:

$$\bar{\sigma} = \bar{\varepsilon}^{p_4} e^{(-p_1 \bar{\varepsilon})} p_2 \sqrt{3} \left(\sqrt{3} \dot{\bar{\varepsilon}} \right)^{p_3} \quad (1)$$

where $\bar{\sigma}$ is the equivalent stress and $\bar{\varepsilon}$ is the equivalent total Von Mises strain. The parameter p_4 is the strain sensitivity, p_3 is the sensitivity of the stress to the strain rate $\dot{\varepsilon}$, p_2 is a proportionality factor and p_1 permits to model softening of the material. These parameters can be fitted on experimental $\sigma - \varepsilon$ curves [Pascon *et al.* 2007].

The second law used here is an elasto-viscoplastic crystal plasticity-based constitutive law written by Y. Huang and modified by J.W. Kysar [Huang 1991]. It takes into account the crystal orientation and the active slip systems. Based on the Schmid law, the slip rate $\dot{\gamma}^{(\alpha)}$ of the α^{th} slip system is determined by the corresponding resolved shear stress $\tau^{(\alpha)}$ by Eqn. (2a), where $\dot{a}^{(\alpha)}$ is the reference strain rate on slip system α , $g^{(\alpha)}$ is a

variable describing the current strength of that system, and n expresses the strain rate sensitivity. The strain hardening is characterized by the evolution of the strengths $g^{(\alpha)}$ through the relation of Eqn. (2b):

$$\dot{\gamma}^{(\alpha)} = \dot{a}^{(\alpha)} \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right)^n \quad \dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)} \quad (2 \text{ a-b})$$

where $h_{\alpha\beta}$ are the slip hardening moduli, the sum ranges over all active slip systems. Here, the hardening matrix is defined by Bassani and Wu [Bassani *et al.* 1991]:

$$\begin{cases} h_{\alpha\alpha} = \left\{ (h_0 - h_s) \operatorname{sech}^2 \left[\frac{(h_0 - h_s) \gamma^{(\alpha)}}{\tau_s - \tau_0} \right] + h_s \right\} G(\gamma^{(\beta)}; \beta \neq \alpha) & ; \quad G(\gamma^{(\beta)}; \beta \neq \alpha) = 1 + \sum_{\beta \neq \alpha} f_{\alpha\beta} \tanh \left(\frac{\gamma^{(\beta)}}{\gamma_0} \right) \\ h_{\alpha\beta} = q h_{\alpha\alpha} \quad (\alpha \neq \beta) \end{cases} \quad (3)$$

where h_0 is the initial hardening modulus, τ_0 , the initial yield stress and also the initial value of $g^{(\alpha)}$, τ_s the saturation stress, h_s the hardening modulus during easy glide within the first stage of hardening and $\gamma^{(\alpha)}$ the total shear strain in slip system α , while “sech” is the hyperbolic secant function. $\gamma^{(\beta)}$ is the total shear strain in slip system β , γ_0 is the amount of slip after which the interaction between slip systems reaches the peak strength, and each component $f_{\alpha\beta}$ represents the magnitude of the strength of an interaction between slip system α and β . The G function implicitly deals with cross-hardening occurring between slip systems during the second stage of hardening [Siddiq *et al.* 2007].

Results: The results using the modified Norton-Hoff constitutive law are given in Fig.2. with the parameters of Table 1. With only one set of parameters, it is not possible to represent the behavior of this material at all strain rates. In fact, one set of parameters can reproduce hardening or softening but not both. The modification of only one parameter for each strain rate is also not sufficient to represent the different behaviors.

For the microscopic constitutive law, a sensitivity analysis on all parameters was done. It reveals that the representation of all the tensile tests of Fig.1. with only the modification of one parameter, h_s , can be done. An h_s evolution law of the type $h_s(\dot{\varepsilon}) = A \ln(\dot{\varepsilon}) + B$ permits to obtain the desired results with an adequate choice of the parameters A and B. This evolution law and the parameters set of Table 2 were validated with one finite element (neglecting effect of grain orientation) and 112 finite elements (taking into account different grain orientations). Results are given in Fig.3.

CONCLUSIONS: Unlike the Norton-Hoff macroscopic law, the microscopic constitutive law modified, the h_s parameter evolution and only one set of parameters model the behavior of the material independently of the strain rate used (constant or not) to perform the test. This law was also used to reproduce a nanoindentation test performed on a β grain of this material. The results are close to the experimental ones.

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Table 1: Norton-Hoff Parameters (100 % β Ti-555)

p_1	3.97517
p_2	1063.8608
p_3	0.011396
p_4	0.183951

Table 2: Microscopic Law Parameters (β – Ti-555).

n	50	τ_0	300	$f_{\alpha\beta i}$	15
$\dot{\alpha}$	0.001	γ_{0i}	0.00091	A	-1.959
h_0	7482	γ_{0ii}	0.000314	B	-14.766
τ_s	304	$f_{\alpha\beta}$	14.6		

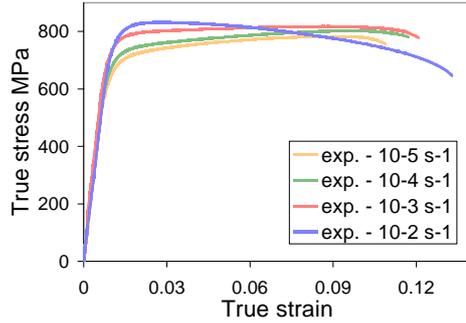


Fig.1 Experimental tensile tests at different $\dot{\epsilon}$ (s^{-1}) on 100% β Ti-555.

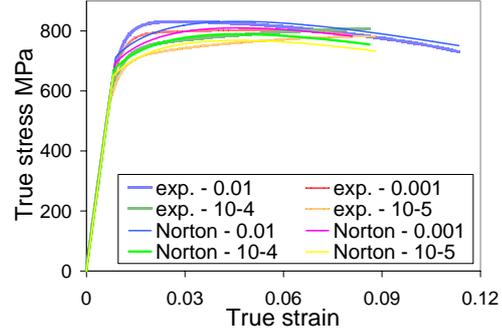


Fig.2 Tensile tests at different $\dot{\epsilon}$ (s^{-1}): Norton-Hoff law, parameters of Table 1.

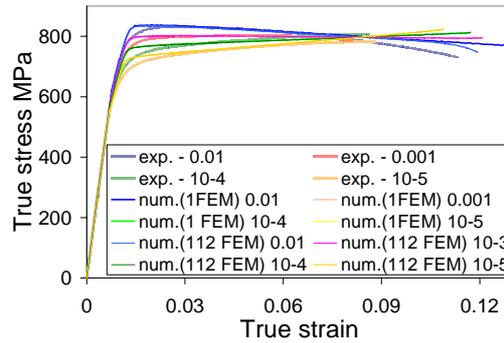


Fig.3 Tensile tests at different $\dot{\epsilon}$ (s^{-1}) on β -Ti-555: microscopic law, h_s evolution and parameters of Table 2.

REFERENCES:

- Bassani J.L., Wu T.Y., 1991, "Latent hardening in single crystals II. Analytical characterization and predictions", *Philos. Trans. R. Soc. London A* **435**, 21-41.
- Huang Y., 1991, "A user-material subroutine incorporating single crystal plasticity in the Abaqus finite element program", internal report, Harvard University, Cambridge.
- Pascon F. Habraken A.M., 2007, "Finite element study of the effect of some local defects on the risk of transverse cracking in continuous casting of steel slabs" *Comput. Methods Appl. Mech. Engrg.* **196**, 2285-2299.
- Siddiq A. *et al.*, 2007, "Fracture of bicrystal metal/ceramic interfaces: A study via the mechanism-based strain gradient crystal plasticity theory", *Int. J. of Plast.* **23**, 665-689.