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NUMERICAL MODELING OF REPRESENTATIVE CELLS OF TI-5553 USING PERIODIC HOMOGENIZATION TECHNIQUE

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Summary. This article focuses on the modeling of representative cells of Ti-5553 using the periodic homogenization theory and a microscopic constitutive law.

1 INTRODUCTION

Ti-5553 is a new generation of Ti alloy suitable for aeronautical applications. Generally, it is composed of a body-centered cubic β-phase and a hexagonal close packed α-phase. Numerical simulations of representative cells using the periodic homogenization theory coupled with the finite element (FE) method (Lagamine FE code, ULg) are performed to optimize its microstructure. The periodic homogenization theory and the microscopic elastic-viscous-plastic (EVP) crystal plasticity-based constitutive law chosen to model the behavior of the two phases of Ti-5553 are first presented. Then, the material parameters and the choice of representative cells are commented. Finally, numerical results are given and discussed.

2 PERIODIC HOMOGENIZATION PRINCIPLE

The studied material is generated by spatial periodicity from a representative cell, ω^0 at an initial time $t=0$. During the structure evolution, the periodic homogenization theory is used[1] to numerically formulate the constitutive equations on the cell ω^t. The macroscopic and microscopic quantities (stress and strain measurements) are linked using the mean relations:

$$L^t = \frac{1}{|\omega^t|}\int_{\omega^t} l^t \, d\omega^t \quad \text{(a)} \qquad ; \qquad \Sigma^t = \frac{1}{|\omega^t|}\int_{\omega^t} \sigma^t \, d\omega^t \quad \text{(b)} \tag{1}$$

where l^t is the velocity gradient, σ^t the Cauchy stress and $|\omega^t|$ the volume of ω^t. With a periodicity assumption for l^t, Eqn. (1 (a)) is equivalent to:

$$l^t = L^t + grad(v^t_{per}) \text{ where } v^t_{per} \text{ is an } \omega^t\text{-periodic velocity field} \tag{2}$$

The virtual power theorem then gives:

$$\forall \delta v^t_{per} : \omega^t \to R^3 \ \ periodic\ on\ \omega^t \quad , \quad \forall \delta L \quad : \quad \int_{\omega^t} (\delta L + grad(\delta v^t_{per})) : \sigma^t \ d\omega^t = \left|\omega^t\right| \Sigma^t : L^t \tag{3}$$

and is obtained using Eqn. (1) and (2), the periodicity of the stress tensor on ω^t, null body forces and the periodicity of the stress tensor on ω^t.

3 CONSTITUTIVE LAW

The set of equations (Eqn. (1) to (3)) must be completed by the constitutive law of the material located in each integration point of some FE discretization of the basic cell ω^t.

For the numerical tests, an EVP microscopic crystal plasticity-based constitutive law written by Y. Huang[2] is used. In this kind of constitutive law, the crystal orientation and the activated slip systems are taken into account. The slipping rate $\dot{\gamma}^{(\alpha)}$ of the α^{th} slip system in a rate-dependent crystalline solid is determined by the corresponding resolved shear stress $\tau^{(\alpha)}$ as

$$\dot{\gamma}^{(\alpha)} = \dot{a}^{(\alpha)} \left(\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}} \right)^n \tag{4}$$

where $\dot{a}^{(\alpha)}$ is the reference strain rate on slip system α and n is linked to the strain rate sensitivity. The strain hardening is characterized by the evolution of the critical resolved shear stresses $\tau_c^{(\alpha)}$ through

$$\dot{\tau}_c^{(\alpha)} = \sum_\beta h_{\alpha\beta} \dot{\gamma}^{(\beta)} \tag{5}$$

where $h_{\alpha\beta}$ are the slip hardening moduli, the sum ranges over all activated slip systems. Here, the hardening matrix is defined by Bassani and Wu[2].

4 MATERIAL AND PARAMETERS

The material used here is Ti-5553 alloy. The parameters[3] of the constitutive law were optimized from experimental macroscopic tests on 100% β material for the β phase and from nanoindentation tests for the α phase.

5 CHOICE AND MODELING OF THE REPRESENTATIVE CELLS

It was decided to model representative cells containing one α grain in a β matrix. The size and shape of the α grain in the matrix were defined from experimental microstructure measurements. The first one is a globular α phase and the second one is an extended α phase. The meshes of the simplified microstructures are given in Figure 1.

A sensitivity analysis was performed in order to study the influence of the appearance of the α phase in the β matrix, the orientation of the α phase, the loading and the shape of the α phase. The orientations are given in Table 1. The difference introduced between the two grain orientations is that the $\vec{c}$ axis of the hexagonal phase is along the global Z direction in the first case and along the Y direction in the second case.

The loading parts are the macroscopic velocity gradients L_1 and L_2. The non-zero components are $L_1(1,1) = L_1(3,3) = -1/2*L_1(2,2) = -0.3$ and $L_2(2,2) = L_2(3,3) = -1/2*L_2(1,1) = -0.3$.

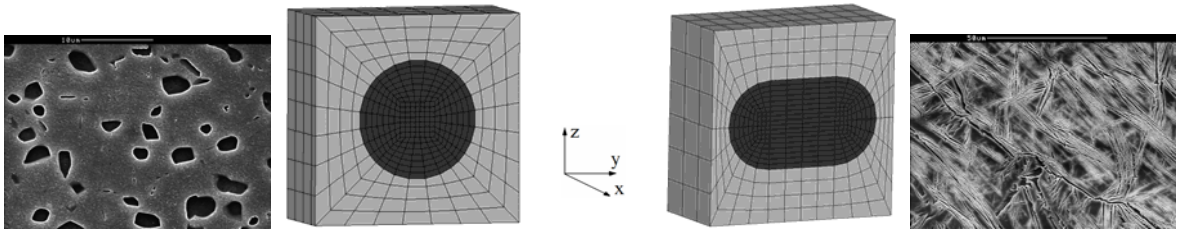

Figure 1: Cross sections of the meshes of the two representative cells chosen from the EBSD pictures. Microstructures 1 (left) and microstructure 2 (right).

Phase	First local axis	First global axis	Second local axis	Second global axis
β	(100)	(100)	(010)	(010)
α (1)	(100)	(100)	(010)	(010)
α (2)	(100)	(100)	(001)	(010)

Table 1: Orientations of the two phases in the global axes.

6 RESULTS AND DISCUSSION

Experimentally, some global tendencies can be observed. Concerning hardness, it was observed[3] that the hardness of the α phase is less than the hardness of the β phase and these are in turn smaller than the hardness of the (α+β) materials. Moreover, it is clear that the ductility of the β material is higher than the ductility of an (α+β) material[4]. For Ti-LCB alloy[4], the ductility of the material composed of lamellar α is less than a material with globular α. Finally, intrinsically, the properties of the lamellar and globular α should be comparable but the characteristic size of the α phase with respect to the deformation mechanism should have an effect on the behavior of the cell. In fact, for example, in a microstructure with a great number of thin lamellar α, boundaries are close to each other and they stop more efficiently the dislocation motion.

The macroscopic Von Mises' stress versus strain results of the representative cell's modeling are shown in Figure 2. In terms of yield point, it is only slightly influenced by the presence and shape of the α phase in the matrix. However, the orientation of the α grain can have an influence on the yield point.

As observed experimentally[3], when the α phase is present within the cell, hardening behavior appears, whereas when only the β phase is present, softening behavior is observed. Results obtained on globular α showed a slight influence of the loading direction but a larger influence of the orientation of the α phase with respect to the β phase. Modifying the orientation or the loading gives another result but the most important remark is that the orientation of the α phase with respect to the loading direction influences the results, beginning from the yield stress. For the lamellar α, it appears that the loading direction strongly influences the results. This conclusion was expected due to the different orientations between the extended α and the loading direction. These results do not give information about ductility, which can be very different from one microstructure to another and which is also an important fact for practical applications.

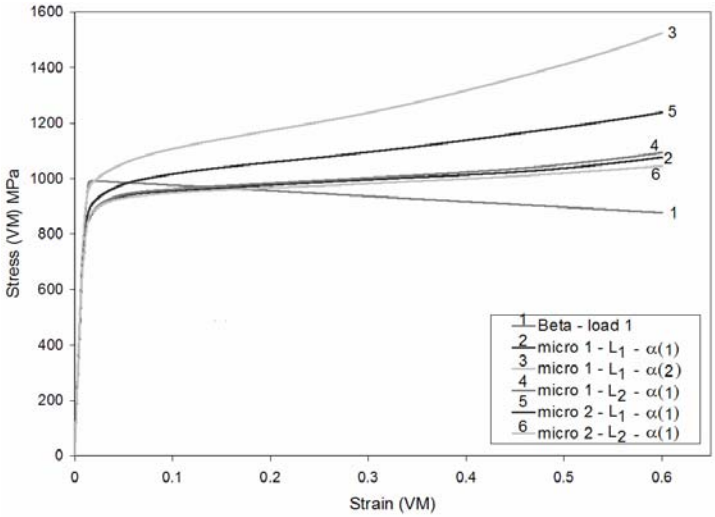

Figure 2: Von Mises' stress versus strain for all the microstructures, loading parts and orientations studied.

7 CONCLUSIONS

This article provided information about the tensile behavior of Ti-5553 using representative cells. To improve modeling of this material, other behavioral aspects need to be studied. For example, the effect of the proportion (the size, the shape and the interdistance of the α phase inside the β matrix) of the α phase inside the β matrix should be investigated. For the same shape, the size of the α phase with respect to the deformation mechanism should have a non-negligible effect on the total behavior of the cell. Moreover, to better model the behavior of the macroscopic material, it may be worthwhile to create representative cells containing several α grains of appropriate orientations. In these cells, the effect of the respective size of the α grains, the relative orientation and the interdistance between them will also be worth investigating. Finally, the addition of interface elements between the α and the β phases should also improve the results.

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