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MULTISCALE MODELLING OF LAMELLAR STRUCTURES: APPLICATION TO γ-TiAl-BASED ALLOYS

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ABSTRACT

A multiscale model for the prediction of plastic behavior of materials with lamellar microstructures is presented and applied to γ-TiAl based alloys formed by polysyntetically twinned (PST) crystals. The model is validated by comparing its predictions with the observed anisotropy of a Ti-48at%Al-2at%Cr as-cast tested under compression.

1. INTRODUCTION

TiAl-based alloys are materials of great technological interest. Besides the experimental efforts to characterize their microstructures and mechanical properties, the interpretation of the experimental data requires a thorough understanding of the basic mechanisms that determine those properties. Micromechanical models for crystal and polycrystal plasticity are, in principle, good candidates for this task but they should be refined in order to account for the complex microstructures often found in these alloys.

Among the variety of microstructures found in γ-TiAl based alloys, the present work is focused on materials having lamellar microstructures. This kind of microstructures (which favors a good creep resistance of the material) can be obtained by appropriate heat treatments or just after casting (Bartels et al. 1995). Especially the as-cast material is expected to be highly anisotropic due to preferred orientations of the lamellar colonies.

A single lamellar colony can be characterized as a polysynthetically twinned (PST) crystal. A PST crystal consists of a single set of lamellae (i.e.: an unique direction of the normal to the lamellar planes can be defined). The crystallography, morphology and strong plastic anisotropy of PST crystals have been described in great detail (see, for instance, Yamaguchi 1991). A PST crystal is formed essentially by γ-TiAl lamellae (tetragonal) and also by few percents of α_2-Ti_3Al lamellae (hexagonal). The orientation relationship between the γ- and α_2-phases is $\{111\}_\gamma // (0001)_{\alpha_2}$ and $<1\bar{1}0]_\gamma // <11\bar{2}0>_{\alpha_2}$ with the basal plane of the α_2-phase being parallel to the habit plane of the lamellae. In the γ-phase there are six different crystallographic orientations which fulfill the above orientation relations. In recent work (Lebensohn et al. 1998) we proposed a simplified model to describe the highly anisotropic plastic behavior of a PST crystal. This model consists in assuming that the PST crystal can be represented by two tetragonal lamellae instead of the complete domain structure and that the influence of the minoritary α_2-Ti_3Al phase can be neglected. For this simplified structure, the model is based on : a) the rate-sensitivity equation to describe crystal plasticity by slip and twinning ; b) the relaxed constraints (RC) theory (Honneff and Mecking 1981) to allow variations of some stress and strain-rate components, according to the morphology of the lamellae and c) the assignment of critical stresses to the slip and twinning systems according to a morphology-based classification.

The aim of the present work is to use this description of PST plasticity as part of a multiscale model for the prediction of the plastic behavior of a γ-TiAl polycrystal with lamellar microstructure, considering it as an aggregate of PST crystals or, briefly, as a *poly-PST-crystal.*

The complex microstructure of such poly-PST-crystal prevents us from using of the most popular large strain micro-macro model, i.e. : the viscoplastic selfconsistent (VPSC) 1-site approach (Lebensohn and Tomé 1993). The main assumption of VPSC 1-site model is that a polycrystal can be regarded as a perfectly disordered aggregate of single crystals which undergo local homogeneous deformation. This scenario does not represent a poly-PST-crystal where local crystallographic, morphologic and topologic correlations between neighbour crystallites do exist and have a non-negligible influence on the overall behaviour of the aggregate. Therefore, instead of the classical two – micro and macro – scales, a proper treatment of these materials requires the definition of three different scales: the microscopic scale, at single crystal (i.e.: a single lamella) level; the mesoscopic scale, at PST crystal level and the macrocopic, at poly-PST-crystal level.

2. MODEL

<u>2.1 Plastic behavior of a single PST crystal</u>. Let us consider the simplified γ-TiAl PST structure, formed by one matrix and one twin. The active deformation modes in γ-TiAl to be considered are: $\{111\}\langle 110]$ ordinary slip, $\{111\}\langle 101]$ super slip and $\{111\}\langle 11\bar{2}]$ twinning (Mecking et al. 1996). If the matrix-twin pair corresponds to a $(\bar{1}\,\bar{1}1)[\bar{1}\,\bar{1}\bar{2}]$ twinning system, it is convenient to adopt a reference frame (called "lamellar axes") having axis x_3^L lying along the twinning direction $[\bar{1}\,\bar{1}\bar{2}]$, axis x_2^L along $[\bar{1}\,\bar{1}1]$ (i.e.: normal to the twinning plane) and axis x_1^L along $[1\bar{1}0]$ (figure 1).

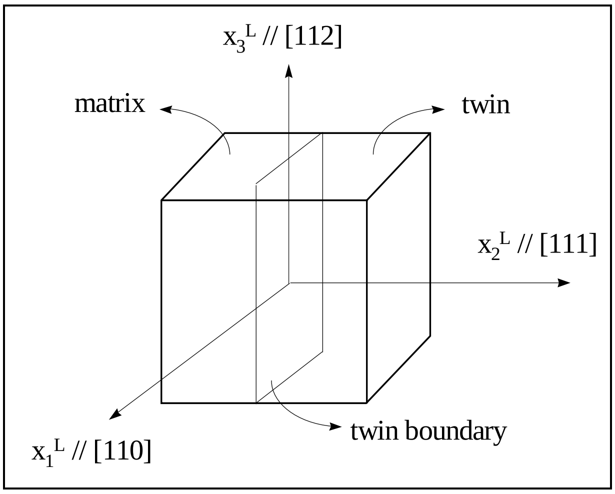

Fig. 1. Definition of the lamellar axes reference frame for a simplified γ-TiAl PST structure.

For each single crystal in this structure, it can be rationally assumed that the morphology determines differences between the critical stresses of deformation systems of the same mode, at very early stages of deformation, i.e.: the critical stress may be different for systems of the same slip or twinning mode depending on the orientation of each system with respect to the lamellar plane. These considerations lead to a *morphology-based* classification of the deformation systems.

In this sense, it is possible to find in each lamella one ordinary slip system, two super slip systems and one twinning system which have their slip (or twinning) direction and slip (or twinning) plane parallel to the interface. These slip (or twinning) systems are grouped in the *longitudinal slip (or twinning) type*. Each lamella also contains one ordinary slip system and two super slip systems with their slip direction parallel to the interface and with the slip plane transversal to the interface. These slip systems corresponds to the *mixed slip type*. Finally, the rest of the ordinary, super and twinning systems have their slip (or twinning) directions and their slip (or twinning) planes transversal to the interface. These slip (or twinning) belong to *transversal slip (or twinning) type*.

Based on the RC theory, when a strain-rate $\bar{\dot{\varepsilon}}_i$ applied to the matrix-twin structure sketched in figure 1, the constitutive relation of the PST structure – in lamellar axes – can be written as:

$$\bar{\dot{\varepsilon}}_i - \dot{\gamma}_o \left(w^M \sum_s m_i^{s,M} \left(\frac{m_j^{s,M} \sigma_j'^M}{\tau_o^{s,M}} \right)^n + w^T \sum_s m_i^{s,T} \left(\frac{m_j^{s,T} \sigma_j'^T}{\tau_o^{s,T}} \right)^n \right) = 0 \quad (1a)$$

$$\dot{\varepsilon}_1^M = \dot{\varepsilon}_1^T \quad (1b)$$

$$\dot{\varepsilon}_2^M = \dot{\varepsilon}_2^T \quad (1c)$$

$$\dot{\varepsilon}_3^M = \dot{\varepsilon}_3^T \quad (1d)$$

$$\sigma_4'^M = \sigma_4'^T \quad (1e)$$

$$\sigma_5'^M = \sigma_5'^T \quad (1f)$$

where: s,M and s,T identify the slip and twinning systems in both lamellae ; w^M and w^T are weight factors proportional to the relative volumes of matrix and twin ; $(\dot{\varepsilon}^M, \sigma'^M)$ and $(\dot{\varepsilon}^T, \sigma'^T)$ are the local states inside the matrix and the twin ; τ_r^s, τ_o^s and m_{ij}^s are the resolved stress, critical stress and the Schmid tensor of system (s), respectively ; $\dot{\gamma}_o$ is a reference strain-rate and n is the inverse of the rate-sensitivity. In (1), the traceless tensors are expressed as 5-dim vectors using a modified (3rd and 4th components interchanged) Lequeu convention. The overall stress in the PST structure can be obtained as:

$$\bar{\sigma}_j' = w^M \sigma_j'^M + w^T \sigma_j'^T \quad (2)$$

2.2 Selfconsistent formulation for a poly-PST-crystal. Regarding each single PST structure inside a poly-PST-crystal as an inclusion embedded in an equivalent medium, it is possible to extend the VPSC 1-site interaction equation (Lebensohn and Tomé, 1993) obtaining, for each PST crystal, the following system of non-linear equations (all tensors expressed in the corresponding set of lamellar axes):

$$\dot{E}_i + \tilde{M}_{ij} \Sigma_j' - \dot{\gamma}_o \left(w^M \sum_s m_i^{s,M} \left(\frac{m_j^{s,M} \sigma_j'^M}{\tau_o^{s,M}} \right)^n + w^T \sum_s m_i^{s,T} \left(\frac{m_j^{s,T} \sigma_j'^T}{\tau_o^{s,T}} \right)^n \right) - \tilde{M}_{ij} \left(w^M \sigma'^M + w^T \sigma'^T \right) = 0 \quad (3a)$$

$$\dot{\varepsilon}_1^M = \dot{\varepsilon}_1^T \quad (3b)$$

$$\dot{\varepsilon}_2^M = \dot{\varepsilon}_2^T \quad (3c)$$

$$\dot{\varepsilon}_3^M = \dot{\varepsilon}_3^T \quad (3d)$$

$$\sigma_4'^M = \sigma_4'^T \quad (3e)$$

$$\sigma_5'^M = \sigma_5'^T \quad (3f)$$

where $(\dot{E},\Sigma')$ is the macroscopic state applied to the poly-PST-crystal and $\tilde{M}$ is the interaction tensor for the PST, defined by:

$$\tilde{M} = (I - S)^{-1} : S : M^{tg} \tag{4}$$

where S is the viscoplastic Eshelby tensor and M^{tg} is the macroscopic tangent compliance which can be obtained by solving iteratively the following selfconsistent equation :

$$M^{tg} = \overline{M}^{tg} : \left(\frac{1}{n}\overline{M}^{tg} + \tilde{M}\right)^{-1} : \left(\frac{1}{n}M^{tg} + \tilde{M}\right) \tag{5}$$

The tangent compliance of the PST structure:

$$\overline{M}^{tg} = \frac{d\bar{\dot{\varepsilon}}}{d\overline{\sigma}} \tag{6}$$

can be calculated writing the RC conditions as follows :

$$\begin{array}{l} K : \left(\dot{\varepsilon}^{M} - \bar{\dot{\varepsilon}}\right) = \overline{\sigma}' - \sigma'^{M} \\ K : \left(\dot{\varepsilon}^{T} - \bar{\dot{\varepsilon}}\right) = \overline{\sigma}' - \sigma'^{T} \end{array} \quad ; \quad K = \begin{bmatrix} \infty & 0 & 0 & 0 & 0 \\ 0 & \infty & 0 & 0 & 0 \\ 0 & 0 & \infty & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{7}$$

Then :

$$d\sigma'^{M} = \left[K : \frac{1}{n}M^{tg,M} + I\right]^{-1} : \left[K : \frac{1}{n}M^{tg,T} + I\right] : d\sigma'^{T} = A : d\sigma'^{T} \tag{8}$$

From (8) is possible to derive :

$$d\bar{\varepsilon} = \left[w^{M}\ M^{tg,M} : A + w^{T}\ M^{tg,T}\right] :\ d\sigma'^{T} \tag{9}$$

$$d\sigma'^{T} = \left[w^{M}\ A + w^{T}\ I\right]^{-1} :\ d\overline{\sigma}' \tag{10}$$

Combining (9) and (10), the PST tangent compliance can be calculated as :

$$\overline{M}^{tg} = \left[w^{M}\ M^{tg,M} : A + w^{T}\ M^{tg,T}\right] : \left[w^{M}\ A + w^{T}\ I\right]^{-1} \tag{11}$$

3. RESULTS

Figure 2 shows the crystallographic and morphologic texture of an as-cast sample of composition Ti-48at%Al-2at%Cr. The lamellae are strongly oriented along direction x_2 of the sample. This material was tested under uncial compression at different angles in the x_2-x_3 plane. The angle ϕ is the tilt angle of the compression axis, measured from x_3 in that plane. For each test, the measured relative yield stresses and the relative transversal strains are shown in figs. 3a and 3b.

The selfconsitent model for poly-PST-crystal plasticity described in the former section was used to reproduce the stress and strain measurements of the as-cast sample. As relative critical stresses we adopted the better combination obtained in a similar fitting procedure performed on a single PST crystal (Lebensohn et al. 1998), i.e. : $\tau_o^{mix} = 2.72\, \tau_o^{long}$ and $\tau_o^{trans} = 3.33\, \tau_o^{long}$. The PST's were assumed to be cigar-shaped ellipsoids elongated in x_2 direction (i.e. : a shape compatible with their actual dendritic morphology).

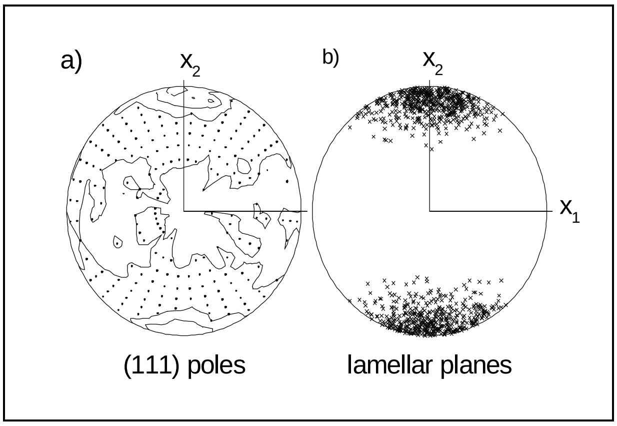

Fig. 2. a) crystallographic b) morphologic textures of as-cast γ-TiAl poly-PST-crystal.

The predictions of yield stresses (relative to the yield stress at φ=90), relative transversal strains and relative activity of the different deformation types are given in figs. 3a, 3b and 3c, respectively. The model predictions show a fairly good agreement with the experiments. The observed yield stress dependence with angle φ (i.e. : relatively low yield stresses at intermediate angles) and the dramatic changes of the relative transversal strain (i.e. : from one kind of plane strain at 0 deg to the opposite plane strain state at intermediate angles to an axially symmetric state at 90 deg) are well reproduced in our calculations.

The plot of the relative activities (fig 3c) shows the role that each deformation type plays at different angles. The hard mixed and transversal slip are specially active at 0 and 90 deg respectively and the more the angle φ deviates from 0 and 90 deg , the less active those hard types become. Consequently, the soft longitudinal slip and twinning types – which accommodate a significant part of the strain, for every orientation of the compression axis – are most active at 45 deg. A similar dependence of the type of active deformation mechanism was obtained with the single PST model by Lebensohn et al. (1998) (in that case, the angle φ was defined by the compression axis and the normal to the lamellar plane) but with extremely sharp changes of the predicted activities: 100% of mixed slip, transversal slip and longitudinal slip and twinning were obtained for 0 deg, 90 deg and intermediate angles, respectively. In the present case, the texture softens that extreme behavior and, due to the local deviations of the lamellar plane orientation, different deformation types are favored in different grains for the same macroscopic orientation of the sample.

4. CONCLUSIONS

The selfconsistent model for the prediction of plasticity of poly-PST-crystals has been validated. The values of relative critical stresses obtained by fitting the results of the single PST model to experiments give also good agreement between model and experiment, when the poly-PST-crystal model is used.

The present model can be use to investigate the anisotropic behavior and texture development of lamellar γ-TiAl alloys of different microstructures, e.g. : grain-shape, volume fraction of lamellar material, etc. under different deformation conditions, e.g. : strain-path, initial texture, strain-rate, etc.

Finally, this multiscale model can be easily extended to deal with other materials having similar highly correlated microstructures.

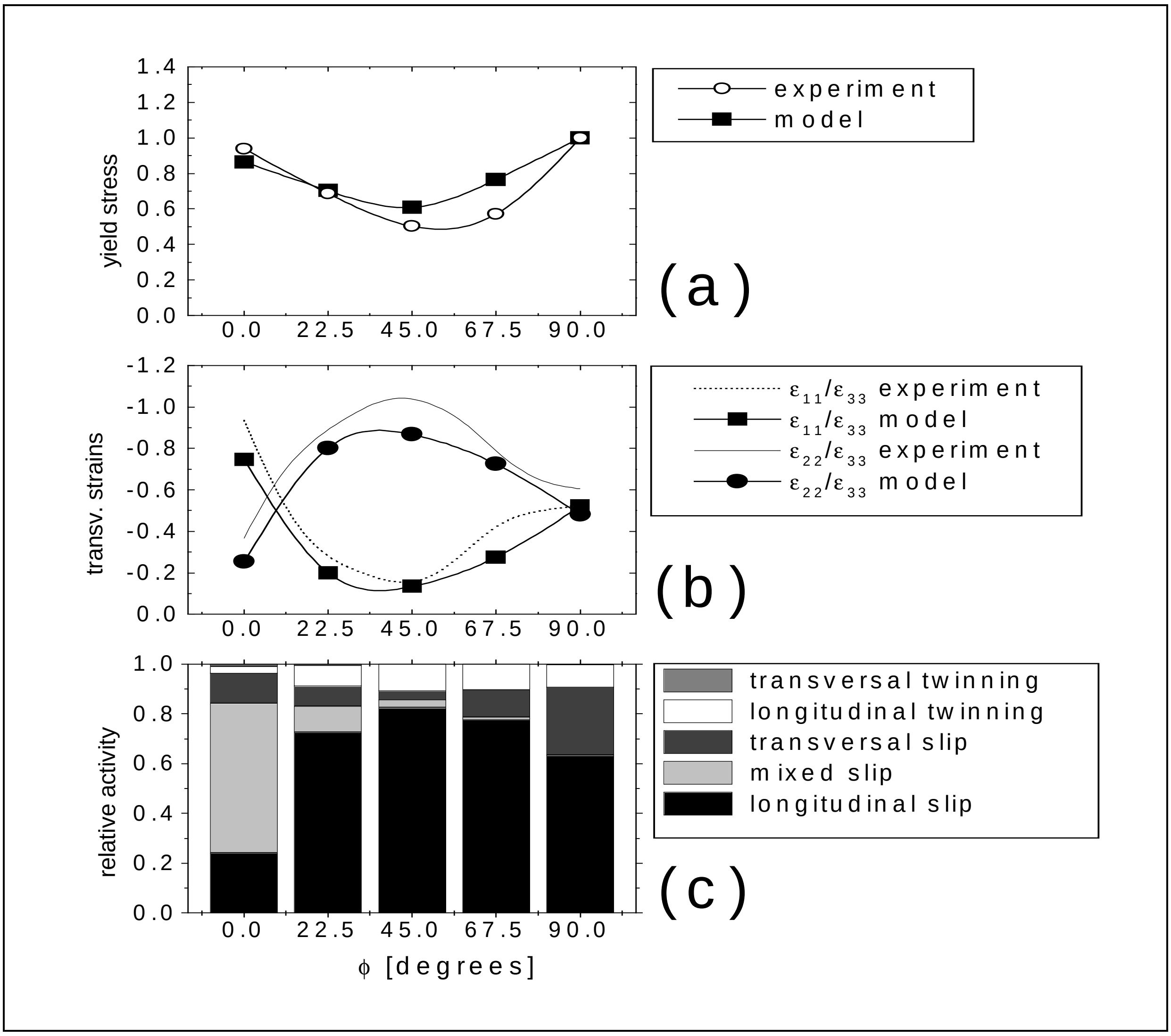

Fig. 3. a) Relative anisotropy of yield stresses : measurements on a Ti-48at%Al-2at%Cr as-cast sample and model predictions. b) Same, for relative transversal strains. c) Relative activities of the deformation types, predicted at different angles ϕ.

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