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MICROSTRUCTURES, ANISOTROPY AND MECHANICAL PROPERTIES OF POLYCRYSTALS: MODELLING STRATEGIES AT DIFFERENT SCALES

Ricardo A. Lebensohn[*], Diego A. González[*], and Javier W. Signorelli[*]

[*] Instituto de Física Rosario (UNR-CONICET)
27 de Febrero 210 Bis - 2000 Rosario, Argentina
e-mail: ricardo@ifir.ifir.edu.ar

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Abstract. *The selfconsistent models for the prediction of the mechanical properties of polycrystals are conceived to account for the influence and evolution of several microestructural aspects like: the anisotropy of the constituent grains, the activity of the different microscopic deformation mechanisms, the volume fraction and the interaction between different phases, the crystallographic and morphologic texture, etc.*

In this work we present the basic equations of the viscoplastic selfconsistent polycrystal model; we show some specific applications to the prediction of: texture development, polycrystal yield surface, intergranular residual stresses; taking into account the effect of: slip geometry, mechanical twinning, recrystallization, grain shape and local correlations and we also discuss the implementation of inverse problem for this kind of formulation.

1 INTRODUCTION

Due to the new characterization techniques which allow to investigate the materials properties and structures down to atomic scale, the development of sophisticated theories and numerical tools for coupling different scales and the increasing numerical capability of computers, the feasibility of multiscale modelling of the mechanical behavior of materials and the interest in its technological applications has been growing in recent years.

Models for the prediction of mechanical behavior of polycrystals are situated at a mesoscopic level, in between the microscopic, ab-initio approaches which take into account the atomic structures of crystalline materials and the macroscopic level, usually solved by means of Finite Elements (FE) techniques. The purpose of this paper is to report on some recent advances in the field of large strain deformation of plastically anisotropic polycrystals. These polycrystal models can be used, in turn, to get the constitutive behavior of each element within a FE calculation. The final aim of such multiscale modelling is to solve a mechanical problem considering not only the geometry and the boundary conditions but also taking explicitly into account the evolution of the microstructure of the material at grain level.

A simple polycrystal theory is the classical Taylor full constraints (FC) model[1] based on the assumption that the local deformation within the polycrystal is homogeneous, meaning that grain of different orientations deform at the same rate. This assumption, which leads to an upper bound for the stress, assures compatibility of deformations but violates stress equilibrium across grain boundaries. The Taylor FC model is not well adapted for materials with high plastic anisotropy. For this reason, the Taylor FC theory has evolved into a new formulation, i.e.: the Taylor relaxed constraints (RC) model[2]. The RC model consists in the complete relaxation of some components of the local strain, based on physical arguments like the grain morphology. This complete relaxation of the strain assumed by the RC theory is an extreme case of the more general viscoplastic selfconsistent (VPSC) approach. The VPSC model is based on treating each grain or a cluster of grains as local viscoplastic inhomogeneities embedded in a Homogeneous Equivalent Medium (HEM) having the same overall viscoplastic response as the polycrystal. In doing this, the both the local strains and the local stresses can be different from the strain and stress state at polycrystal level, depending on the strength of the interaction and the relative anisotropy of each grain and the HEM.

The plan of the paper is as follows: we first present the basic equations of the 1-site VPSC model then we show some specific applications and extensions of this approach involving prediction of texture development, polycrystal yield surface, intergranular residual stresses and taking into account the effect of slip geometry, mechanical twinning, recrystallization, grain shape and local correlations and finally we discuss some aspects of the implementation of inverse problem for the identification of parameters of this kind of formulation.

2 MODEL AND EXAMPLES

2-1 Basic VPSC model

The selfconsistent calculation of the mechanical properties of heterogeneous materials has

been formulated in terms of the Eshelby inclusion formalism[3] by Hill[4] and Hutchinson[5,6]. Later, Molinari et al.[7] developed a general n-sites approach for large strain viscoplasticity and Lebensohn and Tomé[8] implemented the 1-site approximation of Molinari et al model for the calculation of texture development of hcp materials, taking into account the full anisotropy of the polycrystal.

In this section, we present Lebensohn and Tomé's implementation of the 1-site VPSC model. In what follows, $(\sigma';\dot{\varepsilon})$ and $(\overline{\sigma}';\dot{\overline{\varepsilon}})$ denote the deviatoric stress and strain-rate at local (grains) and macrosopic (polycrystal) level, respectively.

If the geometry and critical stresses of the active slip and twinning systems and the orientation of each grain are known, the local strain-rate is given by:

$$\dot{\varepsilon} = \sum_s m^s : \dot{\gamma}^s = \dot{\gamma}_o \sum_s m^s : \left(\frac{m^s : \sigma'}{\tau_o^s} \right)^n \tag{1}$$

where: $m^s, \dot{\gamma}^s$ and τ_o^s are the Schmid tensor, the shear-rate and the critical resolved shear stress (CRSS) of the slip system (s); $\dot{\gamma}_o$ is a reference strain-rate and *n* is the inverse of the rate-sensitivity.

Within the VPSC formulation the stress and strain-rate in the grains can be different from the corresponding macroscopic magnitudes. The deviations of the local magnitudes with respect to the macroscopic ones:

$$\begin{aligned} \tilde{\sigma}' &= \sigma' - \overline{\sigma}' \\ \tilde{\dot{\varepsilon}} &= \dot{\varepsilon} - \dot{\overline{\varepsilon}} \end{aligned} \tag{2}$$

depend on the directional plastic properties of the grains and the whole polycrystal. In order to find this local deviations, each grain is regarded as an viscoplastic inhomogeneity embedded in the HEM. The micro and macro constitutive equations expressed as secant relations are given by:

$$\begin{aligned} \dot{\varepsilon} &= M^{c(sec)}(\sigma'):\sigma' \\ \dot{\overline{\varepsilon}} &= M^{(sec)}(\overline{\sigma}'):\overline{\sigma}' \end{aligned} \tag{3}$$

where the micro modulus can be derived from equation (1) while the macroscopic one is not known a priori but has to be determined selfconsistently.

The VPSC formulation is based on the determination of the interaction tensor $\tilde{M}$, given by:

$$\tilde{M} = n\left(I - S\right)^{-1} : S : M^{(sec)} \tag{4}$$

where S is the viscoplastic Eshelby tensor. This interaction tensor relates the deviations in stress and strain-rate:

$$\tilde{\dot{\varepsilon}} = -\tilde{M} : \tilde{\sigma}' \tag{5}$$

from where it is possible to get the local states. The interaction tensor depends both explicitly and implicitly (via the Eshelby tensor) on the macroscopic modulus. The latter can be determined imposing that the averages of stress and strain-rate over all the grains have to be consistent with the corresponding macroscopic magnitudes. This leads to the following selfconsistent equation:

$$\mathbf{M}^{(\mathrm{sec})} = \left\langle \mathbf{M}^{c(\mathrm{sec})} : \left(\mathbf{M}^{c(\mathrm{sec})} + \tilde{\mathbf{M}} \right)^{-1} : \left(\mathbf{M}^{(\mathrm{sec})} + \tilde{\mathbf{M}} \right) \right\rangle \tag{6}$$

where $< >$ denotes a weighted average over the set of grains.

In order to predict texture development, it is necessary to determine the rotations of the grains. When slip is the only operative mechanism of plastic deformation, the total rotation-rate of grain is given by:

$$\dot{\omega} = \dot{\Omega} - \dot{\omega}^{\mathrm{pl}} + \dot{\omega}^{\mathrm{loc}} \tag{7}$$

where the terms in the right hand are the macro, plastic and local rotation-rates, respectively. The first term (macro) is related with the rigid-body rotation of the polycrystal, if any, while the second one (plastic) can be readily derived from the shear-rates. The third term (local) depends on magnitude of the local deviations in strain and on the assumed grain shape and can be obtained as:

$$\dot{\omega}^{\mathrm{loc}} = \tilde{\dot{\omega}} = \Pi : \mathbf{S}^{-1} : \tilde{\dot{\varepsilon}} \tag{8}$$

where the skewsymmetric Eshelby tensor Π vanishes for spherical grains while its norm increases – and so does the weight of $\dot{\omega}^{\mathrm{loc}}$ in expression (7) – as the grain shape becomes more severe.

2-2 Deformation Twinning

An additional source of rotations is related to twinning activity. When a twin is formed inside a given crystal some volume fraction of it adopts a completely different (but crystallograhically related) orientation. Several schemes has been proposed[9] to deal with the effect of twinning reorientation in texture development. Particularly, for moderate twinning activities (i.e.: when slip participates more than twinning in plastic strain accommodation) the so-called Predominant Twin Reorientation (PTR) scheme has shown to be good enough to capture the main role of twinning reorientation in texture development. The PTR scheme consists in keeping track of the actual sum of individual twinned fractions over all twinning systems and grains and of the effective twinned fraction. This effective twinned fraction is the sum of the volumes of individual grains which are completely reoriented in such a way that this reorientation takes place in those grains and twinning systems which exhibit highest activity throughout the deformation process. The selection algorithm is such that when the actual twinned fraction growths larger than the effective twinned fraction, reorientation by twinning is favoured until the latter catches up. Such procedure is self-controlling and both fractions tend

to remain approximately equal throughout deformation.

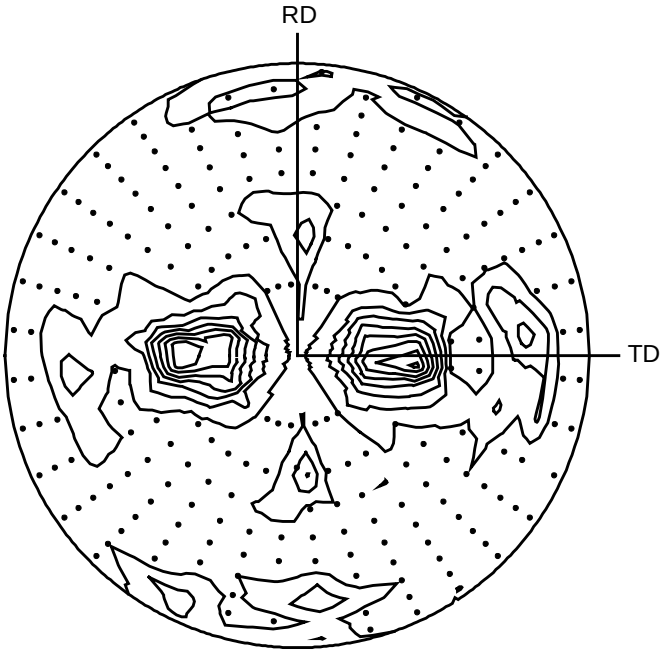

Figure 1: Low Temperature rolling texture (basal poles) of a Zr-alloy predicted with the VPSC model assuming $\tau_{pr} = 1, \tau_{ttw} = 1.25$ and $\tau_{ctw} = 2.5$, after 1.0 Von Mises strain. Lines: multiple of random distribution (mrd). Dots: orientations below 1 mrd.

As an example, figure 2 shows the VPSC prediction of a Zr-alloy rolling texture. At low temperature, Zr-alloys exhibit large activity of $\{10\bar{1}0\}<1\bar{2}10>$ prismatic (pr) slip plus non-negligible presence of $\{10\bar{1}2\}<\bar{1}011>$ tensile (ttw) and $\{11\bar{2}2\}<\bar{1}\,\bar{1}23>$ compressive (ctw) twins. The typical rolling textures of Zr alloys at low temperatures shows a basal maximum in the normal direction - transverse direction (ND-TD) plane, titled 35 degrees from ND[10]. Figure 1 shows the rolling texture calculated with the VPSC model (furnished with the PTR scheme to treat twinning reorientation) starting from random texture, for the following combination of CRSS: $\tau_{pr} = 1, \tau_{ttw} = 1.25$ and $\tau_{ctw} = 2.5$, after 1.0 Von Mises strain. Not just the final texture but also the activity of deformation modes (i.e.: relatively high activity of prismatic slip and low activity of both twinning modes) and the predicted twinned fraction are in good agreement with experimental evidence.

2-3 Recrystallization

In the VPSC formulation some orientations deform more than others leading to large

variations in strain and therefore in stored strain energy. Based on the VPSC model and assuming that the stored strain energy in the grains dominates recrystallization, Wenk et al[11] proposed a deformation-based recrystallization model for low-symmetry materials. From this model, highly strained grains are likely to recrystallize by nucleation or to disappear through invasion by neighbors. Thus, the recrystallization texture is due to a balance between nucleation and the boundary mobility that makes a grain shrink or grow. It should be acknowledged that this recrystallization model inherits an intrinsic limitation from the 1-site VPSC deformation model on which it is based: it assumes that the strain and the strain energy are homogeneously distributed inside the grains. This means that the development of intragranular sources of misorientation and stress concentration (i.e.: potential sites for nucleation of recrystallization) like dislocation structures, twin boundaries, shear bands, etc. is not considered by this model. Nevertheless, making an adequate choice of the nucleation and growth parameters, the model predictions show good agreement with textures observed in experimentally and naturally deformed and recrystallized geological materials, like halite, quartz, ice and calcite[12].

2-4 Polycrystal Equipotential Surface

Unlike a rigid-plastic material, it is not possible to get true yield points (and therefore a true yield surface) of a viscoplastic material. Nevertheless, the relative anisotropy of a viscoplastic material can be estimated by comparing points that belong to the same equipotential surface. This requires to prove the material in a given stress direction and then correct the stress modulus in order to be exactly at the reference potential (i.e.: at the same dissipation-rate). In the limit, when the rate-sensitivity of the viscoplastic material tends to zero, the shape of this equipotential surface tends to the shape of the yield surface of the rate-insensitive material.

The Polycrystal Equipotential Surface (PCEPS) is the locus of stress states associated with an aggregate of grains for different applied strain-rates, at the same dissipation-rate. The PCEPS can be calculated by means of a viscoplastic polycrystalline model and in this way the effect of texture on polycrystal plasticity is taken into account. The PCEPS is built by probing the polycrystal in different strain directions and using a polycrystalline model to obtain the associated average stress over all the grains of the aggregate. The resulting stress defines a point in the 5-dimensional deviatoric stress space belonging to the PCEPS, while the strain vector defines the normal to the PCEPS surface at that point. Hence, for each applied strain tensor, the equation of a plane in the stress space is obtained. The inner envelope defined by the resulting set of planes is a good approximation to the actual PCEPS. Particularly useful is the so-called $\{\pi\}$-projection of the surface in the deviatoric subspace, obtained by projection of the stresses on the deviatoric plane.

As an example, we present here calculations of PCEPS $\{\pi\}$-projections of hcp aggregates at low temperature with different crystallographic textures[13]. Same deformation modes and CRSS as in section 2-2 are assumed. At low temperature, a non centro-symmetric behavior (strength differential) has been observed[14] in textured polycrystals along the predominant <c>-axis texture component. We show here that such effect is associated with the directionality of

twinning and can be well reproduced by the VPSC model. Figure 2 shows the {π}-projection in the axial-tangential plane of the PCEPS calculated for three possible Zr tubes textures having sharp <c>-components along the radial, axial and tangential directions of the tube, respectively plus a random texture case. All curves are normalized to the value of the yield stress for uniaxial tension along the axial direction. The expected strength differential appears clearly. The positive values of yield stresses corresponding to uniaxial tests along the radial, axial and tangential directions are lower than the negative ones, for the radial, axial and tangential textures respectively. In addition, the projection of the random PCEPS is, as expected, a centro-symmetric curve.

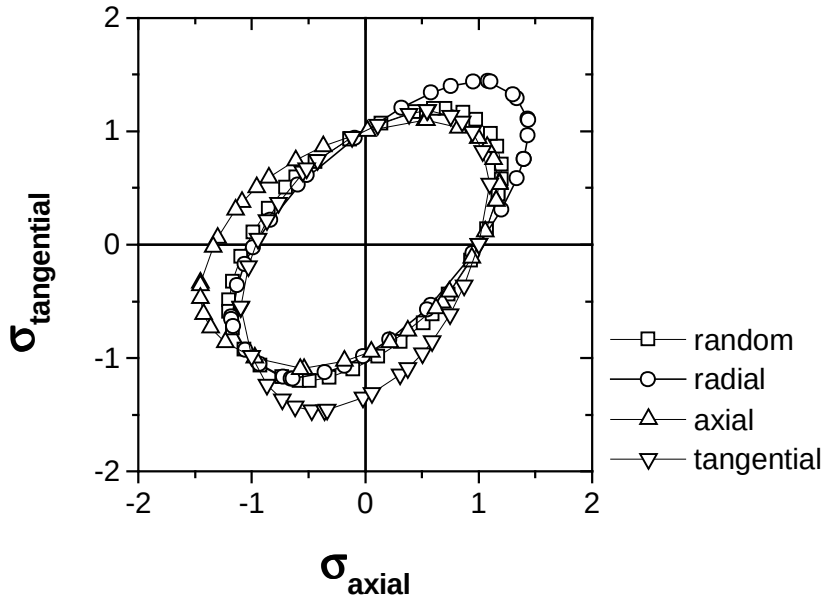

Figure 2: {π}-projection in the axial-tangential plane of the PCEPS calculated with the VPSC model assuming $\tau_{pr} = 1, \tau_{ttw} = 1.25$ and $\tau_{ctw} = 2.5$ for a random texture and Zr tubes textures having the main <c>-component along the radial, axial and tangential directions.

2-5 Intergranular residual stresses

The VPSC model can be extended for the calculation of the intergranular stresses in a polycrystal after large plastic deformation[15,16]. The complete stress state in the grains can be obtained by computing separately the deviatoric and the hydrostatic local deviations with respect to the overall corresponding magnitudes applied to the polycrystal. The extended VPSC model, followed by an elastic selfconsistent unloading has been used to predict intergranular residual states in Incoloy-800 plate after large uniaxial deformation taking explicitly into account the texture evolution and the strain-hardening of the material.

2-6 Local correlations

When different phases are present inside a polycrystal, the spatial distribution of them can be of some importance. Particularly, there are many cases of 2-phases polycrystals for which the vicinity effect between phases is mainly due to a strong correlation in orientation and morphology between neighbour regions of both phases. Furthermore, as the regions of both phases usually form a stack, this correlation is periodically repeated. Therefore, one way to account for the effect of this correlation is to consider two interacting regions of different phases deforming in the HEM by means of a 2-sites VPSC approach[17]. Although we do not present here the complete 2-sites formulation, the essential difference between a 1-site and a 2-sites approaches can be rapidly understood by comparing the shape of the interaction equation. For the 2-sites model the interaction equation is given by (c.f. equation (5) for the 1-site case):

$$\begin{aligned} \tilde{\dot{\varepsilon}}^1 &= -\tilde{M}^{11}:\tilde{\sigma}'^1 - \tilde{M}^{12}:\tilde{\sigma}'^2 \\ \tilde{\dot{\varepsilon}}^2 &= -\tilde{M}^{21}:\tilde{\sigma}'^1 - \tilde{M}^{22}:\tilde{\sigma}'^2 \end{aligned} \tag{9}$$

where the indexes 1 and 2 denote both phases. In (9), the presence of the 2-sites interaction tensors $\tilde{M}^{12}$ and $\tilde{M}^{21}$ indicates that the behavior each site is also affected by the behavior of its neighbour.

Good examples of these kind of correlated 2-phases materials are the lamellar (α+β) Ti alloys. In these alloys, the regions corresponding to one phase are rather flat, and each region of a given phase is always neighbour to a region of the other phase. Their crystallographic orientations are also subjected to certain rules described by the Burgers relation that puts one given crystallographic line and plane of one phase in coincidence with another plane and line of the other phase given by: $\{10\bar{1}0\}_\alpha // \{112\}_\beta$; $<1\bar{2}10>_\alpha // <111>_\beta$ and with the habit plane being the $\{5\bar{1}\bar{4}0\}_\alpha$, near to $\{10\bar{1}0\}_\alpha$ [18].

Figure 3 shows the α-rolling texture (basal poles) after 70% thickness reduction at of a lamellar alloy with 20% β-content, predicted with the 2-sites VPSC model. The active slip modes were assumed to be $\{1\bar{1}0\}<111>$ and $\{11\bar{2}\}<111>$ in the β-phase and $\{10\bar{1}0\}<1\bar{2}10>$ (prismatic), $(0001)<1\bar{2}10>$ (basal) and $\{10\bar{1}1\}<1\bar{2}13>$ (pyramidal) in the α-phase. The first two slip modes (<a>-slip) are assumed to be four times harder than the β-phase slip modes and the latter (<c+a>-slip) eight times harder. The initial texture of each phase was random but such that the neighbour α- and β-orientations fulfill the Burgers relation. This prediction is in good agreement with the experimental rolling textures at intermediate temperatures[19] which exhibit a strong basal component in the transverse direction (TD).

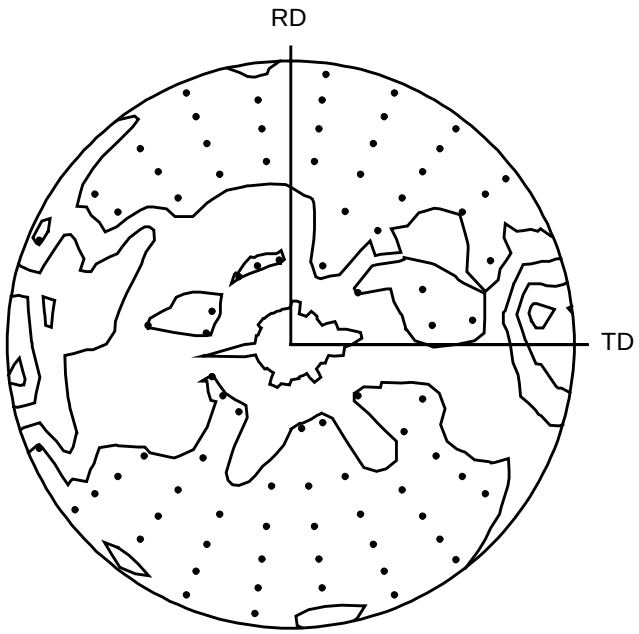

Figure 3: α-rolling texture (basal poles) after 70% thickness reduction of a Ti-lamellar alloy with 20% β-content, predicted with the 2-sites VPSC model.

This good agreement between the actual α-texture and the 2S correlated predictions can be explained in terms of a higher activity of prismatic slip in the α-phase. An increment in the relative prismatic slip activity is indeed observed in the 2S full correlated case, compared with similar 1S results. In the case of lamellar (α+β) Ti alloys, each pair of normal and Burgers vectors of the $\{10\bar{1}0\}<1\bar{2}10>$ prismatic slip mode in the α-phase is parallel to another pair of normal and Burgers vectors of the $\{11\bar{2}\}<111>$ slip mode in the β-phase and these $\{10\bar{1}0\}_\alpha$ and $\{112\}_\beta$ planes are, in turn, almost parallel to the habit plane. Therefore, the simultaneous activation in each phase of these parallel slip systems should be favoured since it makes easier the slip transfer across the interface. This expected increment of prismatic slip activity in the fully correlated case leads to an enhancement of the transverse component in the α-texture since the prismatic slip in hexagonals is known to give rolling textures with a strong basal TD component.

2-7 Inverse problem

Sometimes, the parameters used in the constitutive equations of the VPSC model cannot be measured directly as, for example, the CRSS for slip or twinning of materials for which it is not possible to grow single crystals. In this case, good estimations of these parameters should be done in order to get reliable results from the VPSC model. A systematic determination of the

best set of these parameters requires to couple the polycrystalline model with an optimization scheme[20]. This identification problem is formulated as a sequence of three typical steps: a) definition of an objective function which should express a distance between the simulated and the available experimental textures; b) evaluation of the sensibility matrix for the selected objective function; c) minimization of the objective function with respect to the set of parameters to be determined.

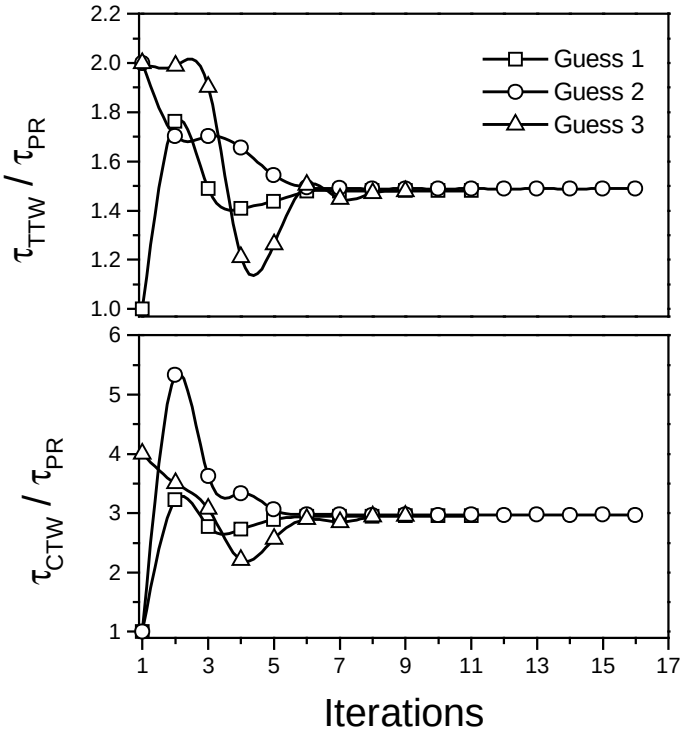

Figure 4: Stability of the identified CRSS values for different initial guesses, assuming as known texture a simulated low-temperature rolling texture of a Zr-alloy obtained with : $\tau_{pr} = 1, \tau_{ttw} = 1.5$ and $\tau_{ctw} = 3$, after 0.6 Von Mises strain.

The objective function is given by a weighted sum of the squares of the differences between corresponding calculated and experimental texture parameters. The objective function can take into account different processes and/or intermediate textures and it may have a regulation term for possible numerical instabilities during the identification calculation. The sensitivity matrix is calculated by analytical differentiation of the direct model equations (see section 2.1) with respect to the whole set of parameters to be identified. This implicit differentiation also contains derivatives of the stress and strain-rate tensors, the micro and macro moduli and the Eshelby tensor. The minimization of the objective function leads to solve a nonlinear system of equations by using a Gauss-Newton algorithm. The minimum of the objective function can be found by an iterative procedure based in a gradient approach plus a linear search algorithm to

find the optimal descendent direction vector for each iteration step. As an example, figure 4 shows the evolution of the identified CRSS until stables values are reached for different initial guesses, assuming as known texture a simulated low-temperature rolling texture of a Zr-alloy obtained with : $\tau_{pr} = 1, \tau_{ttw} = 1.5$ and $\tau_{ctw} = 3$, after 0.6 Von Mises strain.

3 CONCLUSIONS AND PERSPECTIVES

We have shown recent advances in modelling polycrystals with complex microstructructures. Twinning, recrystallization, local correlations in multiphase materials can be considered by means of these kind models. Any of these variants of the VPSC model can be used within a multiscale formulation to get a microstructure-based description of the constitutive behavior at mesoscopic (polycrystal) level. The problem of coupling between crystal and polycrystal models within FE calculations has been extensively investigated in recent years for different regimes of deformation and different scales (for a thorough discussion see Dawson et al.[21]). Among these coupling procedures, the use of the VPSC model has started for large-scale applications in problems involving highly anisotropic materials like forming of Zr-alloys[22] and convection of geological materials[23] in the earth's mantle and inner core.

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