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Polycrystalline models for the calculation of residual stresses in zirconium alloys tubes

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ABSTRACT: Tubes made of different Zirconium alloys are used in various types of reactors. The final texture of tubes as well as the distribution of residual stresses depend on the mechanical treatments done during their manufacturing process. The knowledge and prediction of both the final texture and the distribution of residual stresses in a tube for nuclear applications are of outstanding importance in relation with in-reactor performance of the tube, especially in what concerns to its irradiation creep and growth behaviour. The viscoplastic and the elastoplastic selfconsistent polycrystal models are used to investigate the influence of different mechanical treatments, performed during rolling processes on the final distribution of intergranular residual stresses of zirconium alloys tubes. The residual strains' predictions with both formulations show a non linear dependence with the orientation, but they are qualitatively different. This discrepancy could be explain in terms of the relative plastic activity between the <a>-type and <c>-type deformation modes predicted with the viscoplastic and elastoplastic models.

1 INTRODUCTION

Polycrystalline models for prediction of deformation processes have undergone an important development during the last years. These models allow the prediction of the mechanical behaviour of polycrystals taking into account the effect of the active deformation modes in grains and crystallographic texture. One of the relevant applications of these types of models is to predict the intergranular residual stress field.

In highly plastic anisotropic materials the manufacturing processes lead intergranular residual stresses at the polycrystalline level. These are superimposed to the macroscopic residual stresses and remain in the material when neither applied stress nor macrostresses are present. Later, the residual stresses will affect the response under operation. The polycrystalline models are the most suitable tool to predict the intergranular stress field and to analyze their causes. Among these models, the selfconsistent ones account for grain interactions depending on the relative facility to deform between the grain and the polycrystal. For highly anisotropic materials at single crystal level, as zirconium alloys, a realistic simulation requires the use of selfconsistent formulations.

During the manufacturing process of zirconium alloy tubes, a cold-rolled treatment is applied. This process leads to changes in diameter and thickness of the tube. Each rolling is characterized by the Q-factor, which is defined as the relative variation of the tube thickness and the external diameter. Different values for the Q-factor will give different textures and different residual stresses. We use here both: a viscoplastic selfconsistent model (VPSC) (Hutchinson [1976], Lebensohn and Tomé [1994]) and an elastoplastic selfconsistent model (EPSC) (Hill [1976], Hutchinson [1970]) for the simulation of the rolling process. The first one is used in order to describe texture evolution (high strains and grain rotations) and the intergranular plastic stresses (deviatoric). Under the assumption that the material is elastically isotropic, which holds for zirconium alloys, and assuming that the unloading is purely elastic, the intergranular stresses predicted with the VPSC model could be identified as the residual stresses in the unloading condition. The EPSC model allows to calculate the residual intergranular stresses, but this formulation (small deformations) does not account for the grains rotations. It is used starting from the previous calculated texture (with the VPSC model) and a rolling treatment to small deformation and the corresponding unloading are simulated. This calculation gives the intergranular stresses in the unload condition (deviatoric plus hydrostatic components).

2 THEORETICAL MODELS

In a selfconsistent polycrystalline model each grain (orientation) is considered as an inhomogeneity which deforms embedded in an equivalent homogeneous medium (HEM). This HEM has the overall properties of the polycrystalline aggregate. The key of that type of formulations is to find an interaction equation that relates the stress deviation (grain stress minus polycrystal stress) with the strain deviation (grain strain minus polycrystal strain). This interaction equation is derived using the Eshelby [1957] solution for an inhomogeneity, where the grain is the inhomogeneous inclusion and the HEM is the matrix. From the interaction equation and, with the single crystal and polycrystal constitutive equations, a so called selfconsistent equation for the overall (polycrystal) modulus is derived. This selfconsistent equation is a non-linear equation which can be solved iteratively to find the polycrystral properties as a function of: the single crystal properties, the texture of the aggregate and the grain shape. The solution of this scheme gives the stress-strain state in each grain and the polycrystal (overall) stress-strain, which are a complete characterization of the polycrystalline aggregate response.

In the VPSC formulation the single crystal state is defined by its strain rate and its stress. The strain rate is related to the stress through a potential function (Hutchinson [1976]). In each grain all the deformations modes are active and loading, but their relative contributions depend upon the relation between the resolved shear stress (RSS) over the system and its critical resolved shear stress (CRSS). The selfconsistent solution accounts for the stress dependence of the strain rate locally in the matrix (Lebensohn and Tomé [1994]). In the EPSC model the single crystal state is defined by its strain rate and stress rate. The plastic component to the total strain rate is considered through a Schmid law (Hutchinson [1970]). In this case only a subset of the active modes will be in load and a selection criterium is necessary.

3 RESULTS

In the present work five cases of texture development in zirconium alloys where simulated with the selfconsistent viscoplastic formulation. They correspond to cold-rolled treatments with Q-factors = 0.5, 1.0, 2.0, 4.0 and ∞, and for all the cases the area reduction factor was Ra=65%. Using the reference system sketched in FIGURE 1 (where x_1 is parallel to the rolling direction (RD)), the general case of tube rolling is represented by a macroscopic strain rate that is traceless and has the form:

$$\dot{E} = \begin{Bmatrix} 1 & 0 & 0 \\ 0 & -\dot{E}_2 & 0 \\ 0 & 0 & -\dot{E}_3 \end{Bmatrix}$$

The active deformation modes considered were: prismatic <a> (PR<a>), pyramidal <c+a> (PYR<c+a>), tensile twinning (TTW) and compressive twinning (CTW). The set of Critical Resolved Shear Stress (CRSS) for these system are:

$\tau_{PR<a>} = 1.0$, $\tau_{PYR<c+a>} = 3.5$, $\tau_{TTW} = 1.75$, $\tau_{CTW} = 3.0$

which were setting in units relative to the CRSS of PR<a> systems. Although these values are different from the ones used by Sanchez et al. [1994], we found that the predicted textures (see FIGURE 2) are in reasonable agreement with the previous predictions (Sanchez et al. [1994], Lebensohn [1993]), and with the experimental ones reported by Tenckoff [1978]. The selection of that set of CRSS was made in order to approach not only the previous viscoplastic simulations to obtain the texture development under cold-rolled process, but to have values close to the ones used in calculations of the elastoplastic transition of zirconium alloys textured polycrystals (Turner and Tomé [1994], Turner et al. [1995]). The CRSS for the PR<a> mode was 100 MPa which follows from the comparison between the experimental evidence (loading curve) and the EPSC calculation for the polycrystal yield stress and the elastoplastic transition in Zry 2 sheet (Turner et al. [1995]).

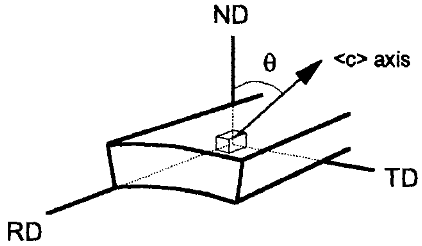

FIGURE 1: Polycrystal reference system in a tube sample.

The grain stresses at the end of the rolling evolution were calculated with the viscoplastic formulation, and also the overall applied stress is known as the average of the grains stresses. The difference (deviation) between the grain stress and the overall stress is approached to the intergranular residual stress. In FIGURE 3 we represent the residual intergranular elastic strains in basal planes for the grains that fulfill the diffracting conditions for different orientations in sample reference system. We choose sample orientations that are in the ND-TD plane, and in the ND-RD plane characterized by the azimuth angle θ (see FIGURE 1).

The residual stress state is explained in terms of the strain boundary condition imposed by the treatment (relate with the Q-factor) and of the relative plastic modes activity. When Q = 0.0 the mechanical treatment is like a transverse pure rolling (the thickness of the tube remains unchanged), for Q = 1.0 the process is a pure tension along RD and Q = ∞ corresponds to a pure rolling. When Q runs from 0.0 to ∞ the relative compressive state between ND-strain and TD-strain runs from more compression along TD to more compression along ND. In the particular case of Q = 1.0 both directions (ND and TD) accommodate the same compressive strain and a uniform straining is supported over ND-TD plane. These boundary conditions and the predictions, from the VPSC model, that the overall plastic activity is mainly prismatic (see TABLE 1) explain the fact that the residual elastic strains over basal planes are tensile for directions close the ND and turns compressive for directions close to the TD when a Q = 0.5 treatment is performed. For the Q = 1.0 the uniform compression over ND-TD plane and the low <c>-type modes activity produced a uniform compressive state for basal directions lying in the ND-TD plane. For Q > 1 the relative compressive final state along ND (to the compression along TD) explains that the <c>-axis were in compression for directions close to the ND and turns tensile for grains which have their <c>-axis close to the TD.

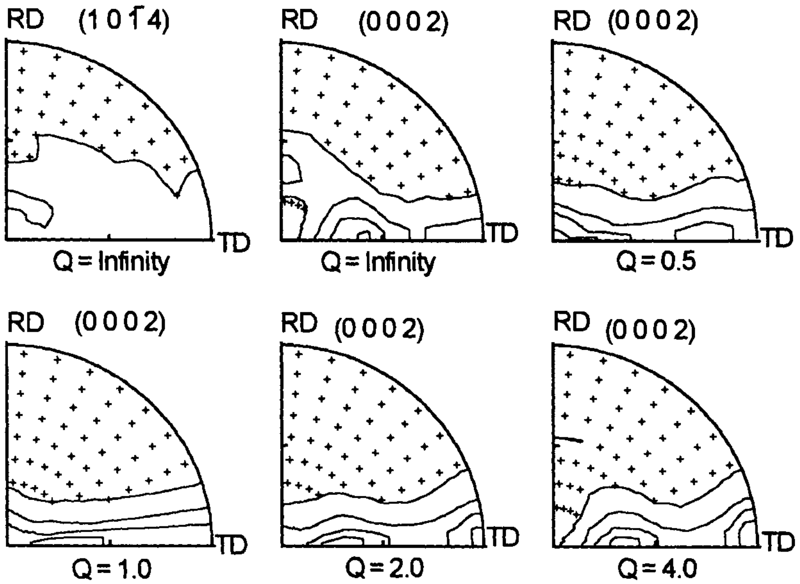

FIGURE 2: Simulated textures with Viscoplastic selfconsistent model. (a)- (1014) pole figure for Q=infinity deformation. (b) to (f)- (0002) pole figures for Q=infinity, 0.5, 1.0, 2.0 and 4.0. (Levels lines in m.r.o.)

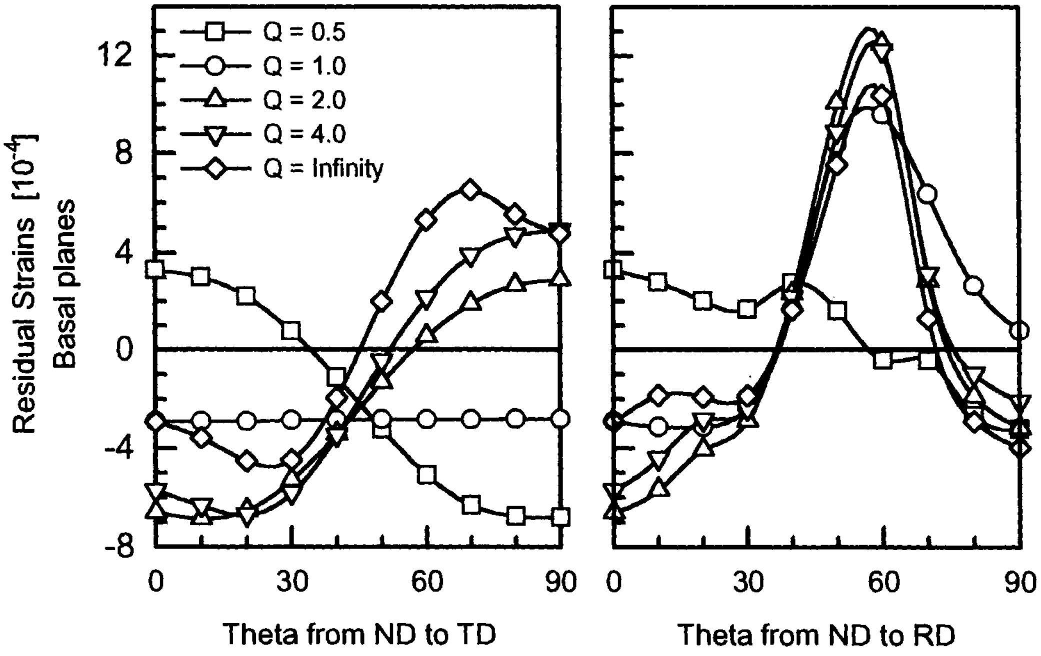

FIGURE 3: Basal planes residual strains for different Q's deformation processes. Predicted with viscoplastic selfconsistent model (VPSC).

	PR<a>	*PYR<c+a>*	*TTW*	*CTW*
VPSC	74.5%	3.0%	10.5%	12.0%
EPSC	44.0%	33.5%	3.5%	19.0%

TABLE 1: Relative activity of deformation modes predicted with both models for the simulation of a rolling treatment (Q-factor = ∞)

The previous analysis also hold for the residual elastic strains over basal planes along directions in the ND-RD plane, but in this case is important to note that a tensile state peak for θ close to 60° appears for all the cases $Q \geq 1.0$. This peak is produced because the grains in such orientations are not favorable oriented to deform by TTW, but in directions closer to the RD the grains can accommodate deformation by TTW (which has a not so high CRSS relative to the PR<a> one). These sets of grains relax the stress state over <c>-planes giving a final compressive state which otherwise must be tensile considering that the boundary condition is tension along RD. This result cannot be easily determined by diffraction measurements because the volume fraction of material that contributes to those diffraction directions is low (see FIGURE 2).

For the limiting case of $Q = \infty$ (pure rolling or channel-die) we performed a simulation of the treatment up to 3% and then unloading using the EPSC model. The polycrystal texture was the one simulated with the VPSC model for the same Q-factor (FIGURE 2) and, the plastic modes and their CRSS' were the same used in the previous calculations. We present in FIGURE 4 the results for the basal planes residual elastic strains in directions lying in the ND-TD plane and in the ND-RD plane. For comparison we also plotted the predictions with the VPSC model. These models give qualitatively different calculations, but this difference is clear from the analysis of the predicted relative plastic activity. While the VPSC model estimates 75% of PR<a> activity and 25% <c>-type modes activity, approximately, the EPSC code calculates 45% PR<a> activity and 55% for the <c>-modes. This indicates that the prediction of the EPSC model is that the plastic deformation is mainly accommodated by PYR<c+a>, TTW and CTW. Then the deformation along <c>-axis will follow the boundary condition, resulting in an inversion of the analysis done for the case of VPSC calculations. Unfortunately, there is not experimental evidence that allows to qualify the predictions between both models. Tomé et al. [1995] report that for Zry 2 sheet after 1.5% channel-die and then unloaded, the basal planes for directions at $\theta = 42°$ from ND to TD are under compression, but our predictions, with both models are close for this direction.

4 SUMMARY AND CONCLUSIONS

- The deformation process produces different textures which have associate different residual strains. The basal plane residual strain for orientations which have their <c>-axis along Normal Direction is tensile for $Q = 0.5$ and is compressive for $Q \geq 1.0$
- The basal plane residual strain distribution for $Q = 1.0$ is uniform with θ from Normal Direction to Transverse Direction. This is a consequence of the fiber texture that presents the deformation process.
- The elastoplastic formulation provides residual strain values opposite to that obtained using the viscoplastic scheme. This result can be explained in terms of the relative activity of prismatic <a> and deformation modes which can accommodate deformation along the <c>-axis (these are pyramidal <c+a>, tensile twinning and compressive twinning).

Even both polycrystalline models are of the selfconsistent type, the constitutive equations for both regimes are quite different. A direct consequence of this fact is the prediction of different activity of plastic deformation modes for a given macroscopic deformation, which induce different residual stresses predictions. Then experimental information is necessary in order to qualify these models.

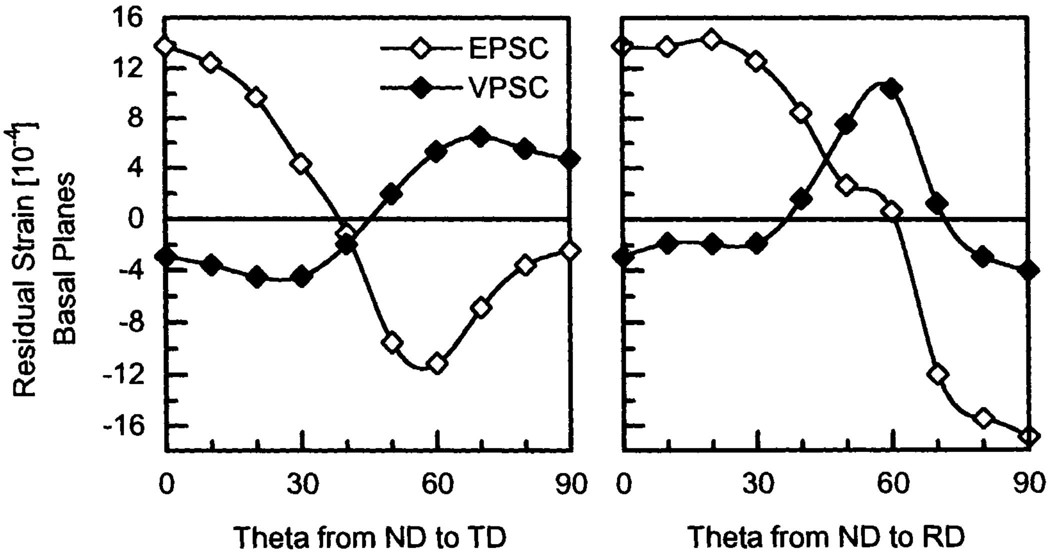

FIGURE 4: Basal planes residual strains for Q=infinity deformation process. Predicted with elastoplastic and viscoplastic models.

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