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David Gloaguen, Marc François, Ronald Guillen. Mesoscopic residual stresses of plastic origin in zirconium: Interpretation of X-ray diffractions results. *Journal of Applied Crystallography*, 2004, 37 (6), pp.934-940. 10.1107/S0021889804022034 . hal-01007026

HAL Id: hal-01007026

<https://hal.science/hal-01007026>

Submitted on 10 Dec 2017

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Mesoscopic residual stresses of plastic origin in zirconium: interpretation of X-ray diffraction results

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Complementary methods have been used to analyse residual stresses in a heat-treated Zr702 sheet which had undergone uniaxial plastic deformation: X-ray diffraction and self-consistent models. The elastoplastic self-consistent model has been used to simulate the experiments and exhibits agreement with experimental data. X-ray diffraction analysis in the rolling direction shows opposite stress values for $\{10\bar{1}4\}$ and $\{20\bar{2}2\}$ planes, respectively. The measured strains were generated by an anisotropic plastic deformation. The comparison between $\varepsilon_{\phi\psi}$ versus $\sin^2\psi$ and simulations confirms that prismatic slip is the main active deformation mode. Plastic incompatibility stress in X-ray measurements should be taken into account in order to make a correct interpretation of the experimental data.

1. Introduction

Like most hexagonal close-packed (h.c.p.) metals, zirconium alloys are elastically, plastically and thermally anisotropic in their properties at mesoscopic (grain) and macroscopic levels (MacEwen *et al.*, 1989; Ortiz & Pochettino, 1996a,b; Turner *et al.*, 1995). When a textured polycrystalline aggregate is subjected to thermo-mechanical treatments, these properties and the crystallographic texture explain the appearance and the development of residual stresses, which may be significant. It is essential to understand the mechanisms responsible for the creation and evolution of internal stresses because their influence on the mechanical performance of the material is usually important.

The purpose of the present work is to combine experimental observations (X-ray diffraction, tensile tests) with the predictions of a self-consistent elastoplastic model in order to obtain more information about the different factors responsible for the appearance of residual elastic mesostrains. This comparison allows a better understanding and interpretation of X-ray diffraction and mechanical results. X-ray diffraction is one of the most commonly used techniques to characterize the mechanical state of polycrystalline materials at the mesoscopic level. It is performed from elastic strain measurements and the subsequent calculation of the stress state by means of mechanics equations. The capacity to measure intergranular strains provides an experimental tool for understanding how intergranular strains are generated. Experimental data from X-ray diffraction offer a rigorous test for the models at a microscopic level (Clausen *et al.*, 1998,

1999; Daymond & Priesmeyer, 2002; Dye *et al.*, 2001; Gloaguen *et al.*, 2002a; Pang *et al.*, 1999).

In a previous paper (Gloaguen *et al.*, 2002b), a study concerning the macroscopic behaviour of rolled textured polycrystalline α -Zr702 after tensile tests has been presented. Self-consistent models were used to simulate the thermal and the tensile response of samples tested along the rolling and the transverse directions (RD and TD) of the sheet. The level and the influence of the thermal stresses on the macroscopic behaviour have been quantified precisely. Results showed that intergranular thermal stresses can affect the macrostress measurement by X-ray diffraction. The slope of $\varepsilon_{\phi\psi}$ versus $\sin^2\psi$ is modified by the thermal residual stresses. It was shown that the thermal stresses can explain the stress differential between the RD and TD of the sample and that the elastoplastic transition can be explained by the texture and the internal stresses. This study enabled us to test the capacity of our model to explain the macroscopic behaviour. The next step is the confirmation of the assumptions regarding the deformation mode in our calculation (the choice of prismatic slip as principal deformation mode). X-ray diffraction stress analysis could constitute an effective validation or identification of a model. For such an analysis, samples are subjected to uniaxial loading with different total strain along the rolling direction. A comparison between stress measurements with the diffraction technique after deformation of these samples and simulation at the mesoscopic level has been achieved. This method permits a better prevision and interpretation of the mechanical behaviour at the different scales (macroscopic, diffracting volume and mesoscopic) of the material. In hexa-

gonal alloys, like zirconium, plastic anisotropy induces plastic incompatibility stresses. These intergranular plastic stresses must be taken into account for a proper interpretation of X-ray experimental data. Consequently, a specific study concerning the influence of these second-order stresses has been performed.

2. Self-consistent scheme

2.1. Theory

The elastoplastic self-consistent model predicts intergranular effects by accounting for the mechanical and thermal anisotropy and the texture of the polycrystal. In this study, we use the self-consistent scheme developed by Hill (1965) and implemented by Hutchinson (1970) to simulate the thermo-mechanical response of polycrystalline aggregates. It is assumed that thermal contractions do not introduce plastic deformation in the material during the cooling process (Ortiz & Pochettino, 1996a,b; Turner *et al.*, 1995). In this case, a thermoelastic formulation is sufficient to simulate the evolution of thermal stresses associated with cooling. The isothermal uniaxial loading is an elastoplastic problem where thermal effects enter through the residual stresses left in the material by the previous cooling process.

The model used for our simulations was presented in a previous paper (Gloaguen *et al.*, 2002b). More details can be found elsewhere (Hutchinson, 1970; Lipinski & Berveiller, 1989). Polycrystal models treat each grain as an inclusion embedded in a homogeneous effective medium (HEM) exhibiting the same overall response of the aggregate. Each grain is considered as an inhomogeneity with elastic (c) and thermal (α) constants, slip and twin mechanisms characteristic of a single crystal. The texture is known; the polycrystal is represented by a weighted discrete distribution of orientations [Euler angles ($\phi_1\phi_2$)]. Lattice rotation (reorientation by slip and twinning) and texture changes are incorporated in the model. However, as expected for such a small strain (<5%), the effect of texture change is negligible.

The stress and strain rates, $\dot{\sigma}^I$ and $\dot{\epsilon}^I$, of each grain are linearly linked by an elastoplastic tensor $\mathbf{I}$. This tensor accounts for the anisotropy of the grains and the hardening effects of the deformation systems during plasticity. The number and type of active systems are defined through their critical resolved shear stress and hardening behaviour. The volume averages of the local stress and strain tensors must coincide with the overall strain and stress, ϵ^I and σ^I . Using the Eshelby inclusion formalism (Eshelby, 1957), $\dot{\sigma}^I$ and $\dot{\epsilon}^I$ of each grain are coupled to $\dot{\sigma}^I$ and $\dot{\epsilon}^I$ through an interaction tensor $\mathbf{L}^*$. It is a function of the Eshelby tensor, the elastoplastic tensor of the polycrystal $\mathbf{L}$, and the shape and the orientation of the inclusion, $\dot{\sigma}^I$ and $\dot{\epsilon}^I$ are linearly linked by $\mathbf{L}$ ($\dot{\sigma}^I = \mathbf{L} \cdot \dot{\epsilon}^I$).

As the properties of the medium are derived from the average response of all grains, $\mathbf{L}$ is initially undetermined and must be solved by iteration. By specifying an overall stress or strain, the model can give the corresponding stress or strain

tensors for each orientation. Thus, we can describe the mechanical response of the polycrystal on the mesoscopic scale.

2.2. Data used in the simulations

For the cooling simulation, we supposed that the sample is stress-free at 923 K (Ortiz & Pochettino, 1996a,b). The texture was introduced in the model by a set of 1000 grains characterized by Euler angles and by weights which represent their volume fraction. The single-crystal elastic constants and the thermal expansion coefficients used in the model are listed by Gloaguen *et al.* (2002b). We take into account the temperature dependence of these coefficients.

For the tensile loading, the temperature is kept constant; the initial internal stresses are those left by the cooling process. The main active slip systems are assumed to be: the six prismatic $\{10\bar{1}0\}\langle 11\bar{2}0 \rangle$ systems, the 24 pyramidal $\{10\bar{1}1\}\langle 11\bar{2}3 \rangle$ systems and $\{10\bar{1}2\}$ twinning. The critical resolved shear stresses (CRSS) used here, $\tau = 118$ MPa for the prismatic mode, $\tau = 190$ MPa for the first-order pyramidal mode and $\tau = 240$ MPa for tensile twinning, give a correct description of the experimental data (Daymond & Priesmeyer, 2002). We considered a linear hardening law (Pang *et al.*, 1999), where the coefficient H^{sr} is equal to H^{sg} for any deformation mode r : $\dot{\tau}^g = H^{sg} \sum_r \dot{\gamma}^r$. The hardening coefficients were found to be 69 MPa for prismatic slip, 150 MPa for pyramidal slip and 240 MPa for twin mode. The CRSS for the prismatic systems is determined to reproduce the experimental yield stress in the RD. The CRSS and hardening coefficients are adjusted to give a good description of the tensile test performed in the RD of the sheet. The same parameters are taken for the simulation of X-ray diffraction results. Fig. 1 shows the predicted stress-strain curves for a tensile test in the rolling transverse direction. The overall comparison between the simulation and the experiment is reasonable. The figure also shows some scattered points representative of the local residual stress/strain state ($\sigma_{11}^I/\epsilon_{11}^I$) for four different macroscopic pre-strains (0, 0.7, 1 and 2%) after elastic unloading. It can be seen that the stress and plastic strain heterogeneity grows with the applied

Figure 1

Experimental (full line) and calculated (dashed lines) macroscopic stress-strain curves for a tensile test in the rolling direction of the sample. Scattered points represent the local strain and internal stress heterogeneity ($\sigma_{11}^I/\epsilon_{11}^I$) for four different macroscopic pre-strains (0, 0.7, 1 and 2%) after elastic unloading. It should be noticed that each point is characterized by a different volume fraction and $\langle \sigma^I \rangle = 0$.

stress. The intergranular plastic strains develop on the mesoscopic scale and vary from grain to grain. Once plastic deformation begins, the original thermal stresses quickly erase. This fact has already been noted experimentally by Pang *et al.* (1999). Fig. 1 shows clearly the role played by the plastic anisotropy. At the beginning (0.7 and 1%), the residual stress/strain state ($\sigma_{11}^I/\varepsilon_{11}^I$) can be represented by a straight line. Prismatic slip is the principal deformation mode. At 2% macroscopic pre-strain, the plastic strain heterogeneity is more important. This phenomenon can be explained by the activation of the pyramidal mode, which becomes more active. The distribution of activated systems is: 52%, 47% and 1% for the prismatic mode, pyramidal mode and tensile twin, respectively.

The next step will be the validation of the assumptions on the deformation modes activated in our calculation. The X-ray diffraction experiments are also simulated with the above parameters to test the validity of these parameters at the mesoscopic level. Both the simulated macroscopic and the microscopic responses are expected to be comparable with experiment. In the study, we determine residual lattice strains in samples with loading to various plastic strains, followed by unloading. In our model, we suppose no plastic deformation during unloading and we consider a purely elastic unloading.

3. Method for the determination of intergranular plastic strains

We present succinctly the principles of residual stress evaluation by X-ray diffraction and the key role played by elastic, thermal and plastic anisotropy properties in the interpretation of the data. More details can be found elsewhere (Baczmanski *et al.*, 1994; Dölle, 1979; Hauk, 1997; Noyan & Cohen, 1987; Ortiz & Pochettino, 1996a,b).

The total elastic strain for a grain at the position X can be expressed in the sample reference S as:

$$\varepsilon(X) = \varepsilon^I + \varepsilon^{II}(X) + \varepsilon^{III}(X). \quad (1)$$

ε^I is the macroscopic strain (first order) averaged over all grains within the macroscopic volume considered. ε^{II} is the intergranular strain (second order) which characterizes the strain deviation from the macroscopic value for a particular grain. ε^{III} is defined as the position-dependent deviations from the average strain of the crystal. Intergranular strains can be present in the material for several reasons.

Elastic anisotropy: the elastic properties of a grain depend on its crystallographic orientation and on the coupling with neighbouring grains. ε^{IIe} is the strain caused by the anisotropy of elastic constants.

Thermal anisotropy: thermal expansion or contraction will depend on crystallographic direction, and elastic strains ε^{IIti} (ti: thermal incompatibility) must be present to maintain compatibility between adjacent grains.

Plastic anisotropy: when a polycrystalline aggregate is subjected to mechanical treatment, the plastic strain in a grain depends on its orientation and those of its neighbours, and large elastic grain interaction ε^{IIpi} (pi: plastic incompatibility)

must develop among the grains in order to maintain strain continuity.

The diffraction method is based on the measurements of the interplanar spacing for various directions of the scattering vector defined by the angles ϕ and ψ (Fig. 2). Diffraction measures the mean interplanar spacing $\langle d(hkil, \phi, \psi) \rangle_{V_d}$ averaged for the diffracting grains that possess a scattering vector normal to the $(hkil)$ plane. The average strain for diffracting grains measured in the x_3^L direction (Fig. 2) can be written as

$$\begin{aligned} \langle \varepsilon'(\phi, \psi, hkil) \rangle_{V_d} &= \frac{1}{V_d} \int_{V_d} (\varepsilon_{33}^{I'} + \varepsilon_{33}^{II'} + \varepsilon_{33}^{III'}) dV \\ &= (\varepsilon_{11}^I \cos^2 \phi + \varepsilon_{12}^I \sin 2\phi + \varepsilon_{22}^I \sin^2 \phi - \varepsilon_{33}^I) \sin^2 \psi + \varepsilon_{33}^I \\ &\quad + (\varepsilon_{13}^I \cos \phi + \varepsilon_{23}^I \sin \phi) \sin 2\psi \\ &\quad + \frac{1}{V_d} \int_{V_d} (\varepsilon_{33}^{IIe} + \varepsilon_{33}^{IIpi} + \varepsilon_{33}^{IIti}) dV \\ &= \frac{\langle d(hkil, \phi, \psi) \rangle_{V_d} - d_0(hkil)}{d_0(hkil)}. \end{aligned} \quad (2)$$

By definition, the mean value of microstrains is zero within each grain and within the diffracting volume V_d .

All quantities defined with respect to the L frame are indicated by prime symbols to distinguish them from those defined in the sample system S. $\langle \dots \rangle_{V_d}$ is the average over diffracting grains for the $hkil$ reflection. d_0 is the stress-free lattice spacing.

In a more synthetic form with the convention $\varepsilon^e(X) = \varepsilon^{IIe}(X) + \varepsilon^I$, the measured strain becomes

$$\langle \varepsilon'(\phi, \psi, hkil) \rangle_{V_d} = \langle \varepsilon^e(\phi, \psi, hkil) \rangle_{V_d} + \langle \varepsilon^{IIti}(\phi, \psi, hkil) \rangle_{V_d} + \langle \varepsilon^{IIpi}(\phi, \psi, hkil) \rangle_{V_d}. \quad (3)$$

If we introduce the diffraction elastic constants $F_{ij}(\phi, \psi, hkil)$ (Dölle, 1979), we can write

$$\langle \varepsilon^e(\phi, \psi, hkil) \rangle_{V_d} = F_{ij}(\phi, \psi, hkil) \sigma_{ij}^I. \quad (4)$$

Finally, equation (3) becomes

$$\langle \varepsilon'(\phi, \psi, hkil) \rangle_{V_d} = F_{ij}(\phi, \psi, hkil) \sigma_{ij}^I + \langle \varepsilon^{IIti}(\phi, \psi, hkil) \rangle_{V_d} + \langle \varepsilon^{IIpi}(\phi, \psi, hkil) \rangle_{V_d}. \quad (5)$$

Figure 2

Sample (S) and laboratory (L) reference system and definition of the angles ϕ and ψ .

Equation (2) or (5) shows clearly that the measured strain cannot be identified as the macroscopic strain if the material presents anisotropic properties. The presence of intergranular strain after a heat treatment and/or a mechanical process influences the measured strain. For example, in a zirconium sample, because of strong thermal anisotropy, the level of residual stress is important after a thermal treatment (Gloaguen *et al.*, 2002b; Ortiz & Pochettino, 1996a,b). The slope of $\langle \varepsilon'(\phi, \psi, hki) \rangle_{V_d}$ versus $\sin^2 \psi$ is not linked to any macroscopic stress; it is a projection of mesoscopic stresses. If these intergranular stresses are not taken into account, the slope determined by X-ray diffraction can be interpreted by mistake as a macrostress of 90 MPa. For a plastic deformation, we have the same problem. Generally, the interpretation of experimental data is based on the unjustified assumption that $\langle \varepsilon'^{I\pi}(\phi, \psi, hki) \rangle_{V_d} = 0$. In our study, we propose to quantify the importance of these intergranular stresses and to show their influence in the interpretation of the experimental results.

After uniaxial loading into the plastic regime, the sample returns to a situation with zero macroscopic stress σ^I , but not with zero lattice strains because of the nonlinear behaviour of the lattice strains and the presence of thermal stresses at the beginning. The measured strain depends only on intergranular strains and has the form

$$\begin{aligned} \langle \varepsilon'(\phi, \psi, hki) \rangle_{V_d} &= \langle \varepsilon'^{I\pi}(\phi, \psi, hki) \rangle_{V_d} + \langle \varepsilon'^{I\pi}(\phi, \psi, hki) \rangle_{V_d} \\ &= \langle \varepsilon'^{I\pi}(\phi, \psi, hki) \rangle_{V_d}. \end{aligned} \quad (6)$$

In our model, the thermal strains arising from the cooling process were calculated with a thermoelastic self-consistent model. The strain and stress tensors of each grain of the polycrystal model are perfectly known before the elasto-plastic deformation. The residual strains calculated are a combination of the initial thermal strains and the intergranular strains generated by the tensile test. The theoretical strain $\langle \varepsilon'^{I\pi}(\phi, \psi, hki) \rangle_{V_d}^{\text{calculated}}$ can be calculated from the self-consistent model and averaged for crystallites having the (hki) normal to the orientation characterized by the ψ and ϕ angles.

For cubic materials, $\langle \varepsilon'(\phi, \psi, hki) \rangle_{V_d}$ versus $\sin^2 \psi$ is not linear but snake-like, owing to the presence of $\langle \varepsilon'^{I\pi}(\phi, \psi, hki) \rangle_{V_d}$ (Baczmanski *et al.*, 1994, 1997; Inal, 1996) (and not only to the presence of elastic anisotropy and crystallographic texture). For zirconium alloys, the measured strains vary quasi-linearly (compared with cubic material) (Cossu *et al.*, 2000; Guillén *et al.*, 1998). We can deduce for each azimuth angle ϕ , the stress value σ_ϕ . Furthermore, σ_ϕ values vary linearly with $\sin^2 \psi$, which means that they are projections of a stress tensor. This result was not self-evident, given the discontinuity of the diffracting volume and its variation with the measurement direction. We can therefore rewrite equation (6) (Cossu *et al.*, 2000):

$$\begin{aligned} \langle \varepsilon'(\phi, \psi, hki) \rangle_{V_d} &= \langle \varepsilon'^{I\pi}(\phi, \psi, hki) \rangle_{V_d} \\ &= F_{ij}(\phi, \psi, hki) \sigma_{ij}^j(hki). \end{aligned} \quad (7)$$

$\sigma^i(hki)$ can be defined as a ‘pseudo-macrostress’ linked to intergranular strain of thermal or/and plastic origin on the diffracting volume. This tensor depends directly on the crystallographic plane. The level and sign values of each component can vary with the level of anisotropy.

The stress tensor σ^i is given by

$$\sigma^i(hki) = \frac{F^i(\phi, \psi, hki) F(\phi, \psi, hki)}{F^i(\phi, \psi, hki) \langle \varepsilon'(\phi, \psi, hki) \rangle_{V_d}}. \quad (8)$$

In the general case, with first- and second-order strains, equation (5) becomes

$$\begin{aligned} \langle \varepsilon'(\phi, \psi, hki) \rangle_{V_d} &= F_{ij}(\phi, \psi, hki) [\sigma_{ij}^I + \sigma_{ij}^j(hki)] \\ &= F_{ij}(\phi, \psi, hki) \sigma_{ij}^{\text{meas}}(hki). \end{aligned} \quad (9)$$

If important intergranular strains are present on the mesoscopic scale in the material after a thermo-mechanical process, the stress tensor $\sigma^{\text{meas}}(hki)$ determined by the usual relation $[F_{ij}(\phi, \psi, hki) \sigma_{ij}^{\text{meas}}(hki)]$ can depend on the analysed family. This behaviour has already been observed by Guillén and co-workers (Guillén *et al.*, 1998; Girard, 1993) on cylindrical Zircaloy-4 samples in the cold-worked state. We have performed a residual-stress analysis using X-ray diffraction. Strain measurements in the tangential and longitudinal directions have been carried out on the $\{10\bar{1}4\}$ and $\{20\bar{2}2\}$ planes. Axial stress analysis showed opposite signs for the two different diffracting planes: 168 MPa and -193 MPa for the $\{10\bar{1}4\}$ and $\{20\bar{2}2\}$ planes, respectively. This measured stress is linked to the sum of strain incompatibilities at the macroscopic and mesoscopic levels. In this case, it is possible to evaluate the magnitude of the first- as well as the second-order residual stresses using equation (5) with a nonlinear fitting procedure associated with a scale transition model (Baczmanski *et al.*, 1994, 1997).

4. Experimental procedure

The investigated material is a commercially pure α -zirconium (Zr702). Its chemical composition is (wt%, balance = Zr): C (0.02), N (0.004), O (0.14) and H (0.0003). The metallographic characterization of the annealed material revealed an average grain size of approximately 20 μm .

4.1. Mechanical testing

Samples of dimensions 2 mm $\times$ 1.5 mm $\times$ 43.4 mm were cut from the rolling direction of the sheet. The specimens were submitted to uniaxial tensile tests at room temperature, at a constant strain rate of $3.8 \times 10^{-3} \text{ s}^{-1}$ up to strains of 0.7, 1 and 2% in the rolling direction. The tensile loading curves are depicted in Fig. 1.

4.2. Stress measurements by the X-ray diffraction technique

We have determined the evolution of internal stresses due to plastic anisotropy in deformed samples after uniaxial loading along the rolling direction. These experiments were carried out on a Siemens D500 goniometer with Cr K α radiation. An Ω goniometric assembly with a scintillation

detector was used. Two plane families were studied: $\{10\bar{1}4\}$ at $2\theta = 156.7^\circ$ and $\{20\bar{2}2\}$ at $2\theta = 137.2^\circ$. Diffractograms were recorded for 15 tilt angles Ψ varying between -45° and 45° , and for azimuth angles $\phi = 0, 45$ and 90° . The direction $\phi = 0^\circ$ corresponds to the rolling direction. The X-ray beam output collimator had a diameter of 0.5 mm and a diffracted-beam slit limited the equatorial divergence to an angle of 0.6° . Peak position is determined by the half-value breadth. The X-ray elastic constants (XREC) $F_{ij}(\phi, \psi, hki\bar{l})$ are theoretically calculated with an elastic self-consistent model. The influence of the texture on these constants is taken into account by weighting single-crystal elastic constants with the texture function. Exemplary plots of F_{11} versus $\sin^2\psi$ for isotropic and textured samples are shown in Fig. 3. Zirconium is mildly elastically anisotropic and the influence of crystallographic texture is relatively weak compared with textured cubic material, such as cold-rolled steel (Baczanski *et al.*, 1993). The curves with rolled texture show small deviations from straight lines. In this case, the XREC can usually be treated as those corresponding to an elastically isotropic material. Only two XREC [$S_1(hki\bar{l})$ and $1/2S_2(hki\bar{l})$] are calculated, in most papers (Hauk, 1997; Ortiz *et al.*, 1993) with the mean slopes and the intercepts of F_{ij} versus $\sin^2\psi$ with anisotropy or isotropic texture (Fig. 3). The stress tensor is calculated by equation (8). We assume a biaxial stress state in the measured region (thin surface layer irradiated by the X-ray diffraction method): σ_{33} is supposed to be equal to 0. The sample shows the typical texture of rolled zirconium. The basal poles are preferentially oriented at an angle of 32° from the normal direction towards the transverse direction, while the prism poles exhibit a weak maximum in the rolling direction.

5. Results and discussion

5.1. X-ray diffraction results

Strains measurements have been performed on two plane families: $\{10\bar{1}4\}$ and $\{20\bar{2}2\}$. In the present section it should be remembered that, owing to the homogeneous macroscopic

Figure 3

F_{11} versus $\sin^2\psi$ calculated values ($\{10\bar{1}4\}$ planes). Filled symbols: isotropic texture; open symbols: experimental texture; triangles: $\phi = 0^\circ$; circles: $\phi = 45^\circ$; squares: $\phi = 90^\circ$.

plastic flow, there is no macroscopic residual stress. The measured and simulated stresses are relative to the diffracting volume, *i.e.* to groups of crystallites with specific orientation. The mentioned stresses are thus ‘pseudo-macroscopic stresses’ $\sigma^{\text{meas}}(hki\bar{l})$ [see equation (9)] associated with intergranular deformation.

To avoid surface effects because of the mechanical history of the sheet or oxygen contamination during the thermal treatment, the specimens were electrochemically polished. Electropolishing was carried out at 298 K under a potential difference of 30 V in a 10% perchloric acid + 90% acetic acid solution. Stress measurements by X-ray diffraction were made at a depth of 100 μm .

Figs. 4 and 5 present the evolution of σ_{11} and σ_{22} of the stress tensor, after unloading, as a function of total deformation (pre-strain) in our samples using the $\{10\bar{1}4\}$ and $\{20\bar{2}2\}$ planes with treatment along the RD. For σ_{11} , the two planes exhibit opposite behaviours: tension for the $\{10\bar{1}4\}$ plane and compression for the $\{20\bar{2}2\}$ plane with a stress value that increases with the amount of pre-strain. At 2% strain, the σ value reaches 143 MPa for $\{10\bar{1}4\}$ and -22 MPa for $\{20\bar{2}2\}$.

Figure 4

Experimental (filled symbols) and predicted (open symbols) evolution of σ with total strain for the $\{10\bar{1}4\}$ plane. Circles: σ_{11} ; triangles: σ_{22} . Axis loading is parallel to the radial direction (RD).

Figure 5

Experimental (filled symbols) and predicted (open symbols) evolution of σ with total strain for the $\{20\bar{2}2\}$ plane. Circles: σ_{11} ; triangles: σ_{22} . Axis loading is parallel to the radial direction (RD).

For σ_{22} , the same behaviour is observed: the stress value reaches 22 MPa for $\{10\bar{1}4\}$ and -67 MPa for $\{20\bar{2}2\}$. X-ray measurements show the effective existence of plastic anisotropy. As can be seen from equation (9), the measured stress depends on a function of the analysed plane family. Strain incompatibilities are present at the mesoscopic level in the material and, consequently, the stresses obtained by X-ray diffraction depend on the plane. The diffracting crystals are not the same for each case, which allows us to deduce that different second-order stresses exist, linked to a strong anisotropic plastic deformation for these two plane families. The same behaviour has already been observed, at large strains, for a cylindrical Zircaloy-4 sample in the cold-worked state (§3).

5.2. Predicted mesoscopic strains

The self-consistent model is also used to simulate the residual intergranular strains (or stresses) after a loading along the rolling direction. The mesoscopic stresses were then averaged and projected on the $\phi\psi$ directions to simulate the X-ray behaviour. Experimental results obtained with X-ray diffraction show that the $\{10\bar{1}4\}$ and $\{20\bar{2}2\}$ planes exhibit opposite stresses. The predicted results agree with the fact that in the $\varepsilon_{\phi\psi}$ versus $\sin^2\psi$ representation of the deformed samples the best fitting for the two studied planes is obtained with prismatic slip as the main deformation mode. In fact, simulations using different combinations of plastic modes (pyramidal or basal slip as the main active deformation mode) were performed and it was found that only the prismatic system can explain the experimental behaviour for all directions ϕ . From equation (9) introduced in §3, it is possible to calculate the theoretical 'pseudo-macroscopic residual stresses' tensor $\sigma^{\text{ic}}_{\text{calculated}}(hkl)$ as a function of total strain for the two studied planes. Figs. 4 and 5 present the evolution of the predicted diagonal components. The agreement between the experiment and the model (with no adjustable parameters) is qualitatively correct. σ_{11} values are opposite for the two studied planes: the stresses associated with $\{10\bar{1}4\}$ are tensile stresses, while compressive stresses are associated with $\{20\bar{2}2\}$. For σ_{22} values, the model gives the correct trends: this component decreases with loading in the RD. However, the amplitude of the simulated stress variation is more important. The residual stresses are overpredicted by the self-consistent model. It is a well known feature of this model (Krier, 1993; Masson *et al.*, 2000; Zaoui & Masson, 2000) which is too 'stiff' because it does not take into account the fluctuations of moduli in the matrix and the inclusion due to the nonlinearity of the mechanical behaviour. Elastoplastic properties are considered as uniform inside the crystallites. The formation of a particular microstructure (dislocation band, wall) inside the crystal is neglected. Discontinuities (grain boundaries, dislocation walls *etc.*) are supposed to have a weak influence on the average behaviour of the aggregate, and dislocation annihilations are not taken into account (Mabelly *et al.*, 1996; Muller, 1994).

Nevertheless, the model allows us to describe the opposite evolution of σ_{11} . It reproduces the fact that the σ_{22} values decrease with the total strain. This behaviour can only be explained with prismatic slip as the main deformation mode and the presence of plastic intergranular strains owing to a strong plastic anisotropy.

6. Conclusions

An elastoplastic self-consistent approach has been developed in order to simulate the mechanical response of rolled Zr under uniaxial loading. Stresses observed by X-ray diffraction are significantly different from one plane family to another. These results can be explained by the presence of mesoscopic stresses of plastic and thermal origin in the material. A self-consistent model has been used to quantify the stress differences between these plane families. The choice of prismatic slip as the principal deformation mode can explain the opposite pseudo-macrostress values for the two studied planes. These predicted results can only be obtained for a single set of slip modes and hardening parameters. This analysis shows that X-ray diffraction stress analysis could constitute an effective validation or identification of a model. Nevertheless, the influence of second-order strain must be taken into account to obtain a correct interpretation of X-ray diffraction results for a hexagonal material.

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