Influence of morphologic texture on stress analysis by X-ray and neutron diffraction in single-phase metallic materials

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Abstract

In this work, a study on the influence of morphologic texture on the residual stress determination by diffraction in metallic materials with cubic and hexagonal symmetry is proposed. To this end, elastic self-consistent model has been developed to properly take into account the morphologic texture. Extreme crystallites morphologies (sphere, disc and fiber) were studied, and coupled with the crystallographic texture to reflect the combined effect of morphologic and crystallographic texture in elasticity. In the case of morphologic texture, a stronger influence than the crystallographic texture on the estimated residual stresses (several tens of MPa difference) was observed. We propose a methodology through a scale transition model to take into account the influence of these different morphologies in the stress analysis by diffraction methods. The main purpose of this work is to make the best choice for lattice planes (hkl) used for residual or internal stress analysis, in elasticity, depending on the morphologic (and crystallographic) texture of the polycrystal, especially when the usual X-ray Elasticity Constants (XECs) are used instead of the stress factors.

1. Introduction

Traditionally, scale transition models proposed by Voigt, Reuss, Neerfeld-Hill or classical Eshelby-Kröner are used [1–8] to describe the distribution of stresses and strains over the oriented grains of a mechanically stressed polycristal. With these models, polycrystalline materials are, in most cases, represented by an isotropic microstructure (equiaxed or spherical grains are considered). Thus, in the absence of crystallographic texture, polycrystals are macroscopically elastically isotropic. This is not generally the case, even in the absence of crystallographic texture.

In crystalline materials, the morphology of the grains is rarely spherical or equiaxed. There are many crystalline materials composed of non-spherical grains with a morphologic texture. One example is the case of thin films with columnar grains investigated in [9–11] using a grain-interaction model combining the extreme Reuss, Voigt, Vook-Witt and inverse Vook-Witt models. Due to the columnar microstructure of these thin films, deviations from an isotropic morphologic microstructure (spherical grains) are observed, thus affecting the macroscopic elastic isotropic behavior of the material as well as the mechanical states experienced by the crystallites. Apart from the thin solid films, there are many others polycrystalline materials that present a microstructure containing non-spherical grains; for example, the structure of the titanium alloy Ti-17 polycrystal consists of needle-shaped α crystallites mixed to slightly equiaxed prior β [12]. Patoor et al. [13] showed *in situ* optical microscopy observations revealing several variants of martensite stress-induced inside each grain of a polycrystalline Cu66.9Zn23.7Al9.4 alloy during uniaxial tensile loading; at high stress levels: induced variants of martensite were strongly oriented by the applied stress. Lacoste et al. [14] investigated amorphous composite materials, made of epoxy resin and carbon-epoxy reinforcing strips, exhibiting an in-plane distribution on the morphologies.

It appears obvious that polycrystals with a morphologic texture have macroscopic anisotropic properties even in the absence of crystallographic texture. The modelling of the mechanical behavior of metallic polycrystals with an anisotropic microstructure can be carried out by deductive methods based on strain mechanisms and scale transition methods like the Eshelby-Kröner self-consistent model. This kind of micromechanical modelling seems to be particularly well suited to describe the material evolution [15–17]. When dealing with scale transition techniques, the internal structure of the material is introduced into the model and its evolution rules are derived from the governing field equations. The grain is used as a basic element representing this structure. It is characterized by its shape, position and orientation defining the morphologic texture. Generally, for the needs of the numerical simulation, each grain is considered as a uniform entity with uniform stress and strain fields.

On the other hand, diffractions experiments provide information about the mechanical stresses of elastic and plastic origin (this latter is not discussed here). Using X-ray or neutron diffraction as an analytical tool, the change in the lattice parameters due to strain occurrence is measured through the induced diffraction peak shift in order to determine the internal stresses. The X-ray Elasticity Constants (XECs) which correlate the measured strains as measured by diffraction with the stress tensor components may be calculated with a suitable grain-interaction model like the Eshelby-Kröner self-consistent model. Strictly speaking, in the case of elastically macroscopically anisotropic materials, XECs cannot be used; diffraction stress factors must be applied. Because the stress factors are much more difficult to determine than the XECs, experimentally as by modelling, XECs are often used instead of the stress factor [18–22]. Thus, significant deviations between the real stress state and the one determined experimentally by diffraction methods may occur. These deviations will vary according to the analysed (*hkl*) lattice plane due to the dependence between the stress factors and the lattice planes.

The aim of this paper is to demonstrate and quantify the influence of the morphologic or/and crystallographic texture on the mechanical properties. Special attention is paid to the determination of macroscopic stress of elastic origin and show the influence of the extreme anisotropy induced by grain-shape in the context of stress analysis by diffraction methods: X-ray diffraction (XRD) or neutron diffraction (ND). We are interested in the $\varepsilon_{\varphi\psi}$ versus $\sin^2\psi$ distributions and stress states which are traditionally deduced. We will quantify these deviations for a large set of (*hkl*) lattice planes and materials with different symmetries (cubic and hexagonal). Eventually, the best choice of the (*hkl*) lattice planes according to the morphologic texture of the material will be proposed. The accuracy of the simulations is evaluated by referring to mechanical experiments (tensile tests and XRD) which were previously published.

2. Eshelby-Kröner self-consistent modelling

2.1. Accounting for an extreme morphologic texture through the self-consistent model

Eshelby-Kröner self-consistent model, used in this study, is a very relevant model for describing the elastic behavior of crystalline materials. Indeed, it predicts more accurately the interactions and effects of intergranular heterogeneities than estimates such as Reuss, Voigt or Neerfeld-Hill approximations, as an example. Apart from the materials consisting of equiaxed grains, a grain-shape texture can also be incorporated in the Eshelby-Kröner approach by considering ellipsoidal inclusions, provided that they have the same orientation in the specimen (as shown in Fig. 1). Even if it is not discussed in this paper, note that this model is also able to account for the influence of a free surface (anisotropic interaction between grains located in the near-surface of the sample), assuming, in particular that grains of the subsurface can be freely deformed in the normal direction. For details, the reader is referred to [23, 24].

To calculate the polycrystalline elastic constants from the single-crystal data assuming the approach developed by Eshelby [3] and Kröner [4], the crystallites surrounding a considered individual grain in a polycrystal are conceived as an elastically homogenous matrix with the elastic properties of the entire polycrystal. The local strain (at the grain scale) $\boldsymbol{\varepsilon}^{II}$ and stress $\boldsymbol{\sigma}^{II}$ can be obtained classically through the strain localization $\boldsymbol{A}$ and stress concentration $\boldsymbol{B}$ tensors:

$$\boldsymbol{\varepsilon}^{\boldsymbol{II}}(\boldsymbol{\Omega}) = \left[\boldsymbol{I} + \boldsymbol{E} : (\boldsymbol{c}(\boldsymbol{\Omega}) - \boldsymbol{C})\right]^{-1} : \boldsymbol{\varepsilon}^{\boldsymbol{I}} = \boldsymbol{A}(\boldsymbol{\Omega}) : \boldsymbol{\varepsilon}^{\boldsymbol{I}} \quad (1)$$

$$\boldsymbol{\sigma}^{\boldsymbol{II}}(\boldsymbol{\Omega}) = \boldsymbol{c}(\boldsymbol{\Omega}) : \left[\boldsymbol{I} + \boldsymbol{E} : (\boldsymbol{c}(\boldsymbol{\Omega}) - \boldsymbol{C})\right]^{-1} : \boldsymbol{C}^{-1} : \boldsymbol{\sigma}^{\boldsymbol{I}} = \boldsymbol{B}(\boldsymbol{\Omega}) : \boldsymbol{\sigma}^{\boldsymbol{I}} \quad (2)$$

where $\boldsymbol{c}$ and $\boldsymbol{C}$ are respectively the mesoscopic and the macroscopic stiffness tensors; $\boldsymbol{I}$ represents the fourth order identity tensor. $\boldsymbol{\varepsilon}^{\boldsymbol{I}}$ and $\boldsymbol{\sigma}^{\boldsymbol{I}}$ are respectively the average strain and stress of the polycrystal. $\boldsymbol{A}$:$\boldsymbol{B}$ denotes the double scalar product $A_{ijkl}B_{klmn}$ using the Einstein summation convention. We describe the orientations of a crystallite within a polycrystalline sample by specification of the rotations $\boldsymbol{\Omega}$ (φ_1, ϕ, φ_2) which relate the sample to the crystal referential system. φ_1, ϕ, φ_2 are the three Eulerian angles [25]. The Orientation Distribution Function (ODF) [26] is used to give a quantitative description of crystallographic texture. The ODF indicates the volume fraction of grains with a certain orientation $\boldsymbol{\Omega}$. $\boldsymbol{E}$ is the so-called Morris tensor, which expresses the interaction between an inclusion (grain) with a given morphology and the Homogeneous Equivalent Medium (HEM). The Morris tensor $\boldsymbol{E}$ can be calculated for the case of an ellipsoidal inclusion (grain) shape as follows [25, 27]:

$$E_{ijkl} = \frac{1}{4\pi} \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} \gamma_{ikjl} d\phi = S_{ijkl}^{Esh} C_{ijkl}^{-1} \quad (3)$$

with

$$\gamma_{ikjl} = K_{ik}^{-1}(\boldsymbol{\xi}) \xi_j \xi_l \quad (4)$$

$$K_{jp}(\boldsymbol{\xi}) = C_{ijpl} \xi_i \xi_l \quad (5)$$

$$\xi_1 = \frac{\sin\theta \cos\phi}{a_1}, \quad \xi_2 = \frac{\sin\theta \sin\phi}{a_2}, \quad \xi_3 = \frac{\cos\theta}{a_3} \quad (6)$$

where $\boldsymbol{S}^{\boldsymbol{Esh}}$ is the Eshelby tensor; the a_i are the lengths of the principal axes of the ellipsoid, used to describe grains shape.

2.2. Application of Eshelby-Kröner self-consistent model to stress analysis by diffraction

Diffraction methods like the $\sin^2\psi$ method [8] for determining residual or internal stresses in polycrystalline materials are based on the measurement of the lattice spacing of the (*hkl*) planes in crystallites composing the diffracting volume. The diffraction geometry is shown in Fig. 2. The irradiated surface of the investigated specimen is perpendicular to its normal direction (S_3 axis). The direction of the strain measurement, i.e. the direction of the diffraction vector **n**, is usually identified by the φ and ψ angles, where ψ is the declination angle and φ denotes the rotation of the specimen around the specimen surface normal; it is the angle between the longitudinal direction (S_1 axis) of the sample and the projection $L_1^{'}$ of the diffraction vector to its surface. $L_1^{'}$ is the stress measurement direction. (L_1, L_2, L_3) is the laboratory frame of reference. This frame is chosen in such a way that the L_3 axis coincides with the diffraction vector in the diffraction experiment. The diffraction vector **n** is the normal of the reflecting lattice planes; it can be expressed in the specimen frame of reference by:

$$\mathbf{n}(\varphi,\psi)=\begin{pmatrix}\sin\varphi\cos\psi\\ \sin\varphi\sin\psi\\ \cos\psi\end{pmatrix} \tag{7}$$

The elastic lattice strain $\varepsilon_{\varphi\psi}$ of a grain group having common (*hkl*) plane-normal, parallel to the diffraction vector **n** (i.e. grains fulfilling diffraction conditions) can be calculated from measured lattice spacing $\langle d(\varphi,\psi,hkl)\rangle_{V_d}$ and a reference one $d_0(hkl)$ using the following expression:

$$\varepsilon_{\varphi\psi}=\ln\left(\frac{\langle d(\varphi,\psi,hkl)\rangle_{V_d}}{d_0(hkl)}\right) \tag{8}$$

where d_0 is the strain-free lattice parameter of the (*hkl*) planes. $\langle\ \rangle_{V_d}$ indicates an averaging over diffracting grains for the considered *hkl* reflection.

$\langle d(\varphi,\psi,hkl)\rangle_{V_d}$ is calculated using the well-known Bragg's law once 2θ angle has been determined form measured diffraction peak. The strain in the **n** direction is then given by:

$$\varepsilon_{\varphi\psi}=\ln\left(\frac{\sin\theta_0(hkl)}{\sin\theta(\varphi,\psi,hkl)}\right) \tag{9}$$

where θ_0 is the Bragg angle of the stress-free material.

The elastic lattice strain $\varepsilon_{\varphi\psi}$ measured by diffraction can also be calculated as the average second order lattice strain over diffracting grains for the considered (*hkl*) plane in the **n** direction:

$$\varepsilon_{\varphi\psi}=\left\langle\varepsilon^{II}(\varphi,\psi,hkl)\right\rangle_{V_d}=\mathbf{n}(\varphi,\psi).\left\langle\boldsymbol{\varepsilon}^{\boldsymbol{II}}(\boldsymbol{\Omega})\right\rangle_{V_d}.{}^t\mathbf{n}(\varphi,\psi) \tag{10}$$

where ${}^t\mathbf{n}$ is the transpose of **n**.

By using Eshelby-Kröner formalism (Eq. 1), this equation is rewritten as follows:

$$\varepsilon_{\varphi\psi}=\left\langle\varepsilon^{II}(\varphi,\psi,hkl)\right\rangle_{V_d}=\mathbf{n}(\varphi,\psi).\left\langle\left[\boldsymbol{I}+\boldsymbol{E}:(\boldsymbol{c}(\boldsymbol{\Omega})-\boldsymbol{C})\right]^{-1}\right\rangle_{V_d}:\boldsymbol{\varepsilon}^{\boldsymbol{I}}.{}^t\mathbf{n}(\varphi,\psi) \tag{11}$$

In the general case of crystallographically or/and morphologically textured material, the dependence of the measured lattice strains on the averaged stresses over diffracting grains is described by the main relationship for stress analysis, using the X-ray stress factors F_{ij} [8, 28–30]:

$$\varepsilon_{\varphi\psi} = F_{ij}\left(\varphi,\psi,hkl\right)\sigma_{ij}^{I} \tag{12}$$

Experimentally, stress factors are evaluated by an uniaxial tensile or bending test. It can also be predicted using the single crystal data coupled with the orientation distribution function (or grains shape in the case of morphologic texture) after adopting a suitable grain-interaction model [8, 26, 31, 32].

For non-textured materials, the stress factors F_{ij} stand for a combination of the XECs, ½S_2(*hkl*) and S_1(*hkl*):

$$F_{ij}\left(\varphi,\psi,hkl\right) = \frac{1}{2}S_2\left(hkl\right)n_i\left(\varphi,\psi\right)n_j\left(\varphi,\psi\right) + S_1\left(hkl\right)\delta_{ij} \tag{13}$$

where δ_{ij} is the Kronecker symbol. By using this latter, Eq. 12 becomes, for a non-textured, macroscopically isotropic polycrystalline material (with homogeneous macroscopic elastic properties):

$$\varepsilon_{\varphi\psi} = \frac{1}{2}S_2\left(hkl\right)\left(\sigma_{\varphi}^{I} - \sigma_{33}^{I}\right)\sin^2\psi + \frac{1}{2}S_2\left(hkl\right)\tau_{\varphi}^{I}\ \sin 2\psi + S_1\left(hkl\right)Tr\left(\boldsymbol{\sigma}^{I}\right) + \frac{1}{2}S_2\left(hkl\right)\sigma_{33}^{I} \tag{14}$$

where

$$\sigma_{\varphi}^{I} = \sigma_{11}^{I}\cos^2\varphi + \sigma_{12}^{I}\sin 2\varphi + \sigma_{22}^{I}\sin^2\varphi \tag{15}$$

and

$$\tau_{\varphi}^{I} = \sigma_{13}^{I}\cos\varphi + \sigma_{23}^{I}\sin\varphi \tag{16}$$

σ_{φ}^{I} and τ_{φ}^{I} are, respectively, the normal stress and the shear stress in the φ-direction. XECs can be calculated by modeling the behavior of the non-textured polycrystalline aggregate. These quantities are also available from experimentations.

By considering a tensile test along the axis S_1 (with $\varphi = 0°$), Eq. 12 becomes:

$$\varepsilon_{\varphi\psi} = F_{11}\left(0°,\psi,hkl\right)\sigma_{11}^{I} = \frac{1}{2}S_2\left(hkl\right).\sigma_{11}^{I}\ sin^2\psi + S_1\left(hkl\right).\sigma_{11}^{I} \tag{17}$$

$\varepsilon_{\varphi\psi}$ plotted versus $\sin^2\psi$ for isotropic polycrystalline materials is therefore a straight line. Its slope is proportional to σ_{11}^{I}. By simulating an uniaxial tensile test with a macroscopic stress σ_{11}^{I} = 100 MPa, we calculated first the ½S_2(*hkl*) and S_1(*hkl*) XECs for several polycrystals with cubic or hexagonal symmetries (aluminum, beryllium, copper, zirconium, titanium, cadmium, alpha-iron and gamma-iron) consisting of 20000 equiaxed grains with random crystallographic orientations. This choice of 20000 grains will enable to have a large number of diffracting grains, and therefore, high-accuracy on the calculated XECs. The XECs obtained are in good agreement with constants obtained numerically in [8, 33] and experimentally in [31, 32, 34].

As we will see in the following, texture effects on stress analysis by diffraction methods are very low when the individual crystallites of a polycrystal are quasi-elastically isotropic. For this reason, only the results obtained for the zinc and the gamma-iron which single crystals are strongly elastically anisotropic will be presented in this paper. Table 1 gives XECs calculated for these two materials, using 20000 equiaxed grains with random crystallographic orientations. The single-crystal elastic constants used in the simulations are: c_{11} = 197.5 GPa, c_{12} = 124.5 GPa, c_{44} = 122.0 GPa for the gamma-iron [35] and c_{11} = 163.7 GPa, c_{12} = 36.4 GPa, c_{13} = 53.0 GPa, c_{33} = 63.5 GPa, c_{44} = 38.8 GPa, c_{66} = 63.6 GPa for the zinc [36, 37].

Fig. 3 shows, for $\varphi = 0°$, $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams for the (200) and (220) lattice planes of the gamma-iron (γ-Fe), (00.4) and (10.4) of the zinc, in the absence of morphologic and crystallographic textures. One can observe a straight evolution of the average lattice strains. The vertical bars or rows of points in this figure indicate the second order lattice strains distribution at a given inclination angle ψ. This second order lattice strains distribution is due to the elastic anisotropy of the crystallites constituting the diffracting volume.

In the remainder, we will distinguish two cases of simulation of $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams: XRD and ND. In XRD, these diagrams are simulated with 21 tilt angles ψ ranging from -60 to 60°. They were simulated, in ND, with 31 tilt angles ψ varying between -90 and 90°. These are typical values used, respectively, in XRD and ND measurements [8].

3. Influence of morphologic texture on stress analysis by diffraction

Taking into account an extreme morphologic texture will influence the macroscopic elastic behavior of the polycrystal (the corresponding macroscopic elastic behavior of which is obviously transversely isotropic). Indeed, as one can observe from Eq. 10, a modification of second order elastic lattice strains $\boldsymbol{\varepsilon^{II}}$ would influence the measured elastic lattice strain $\varepsilon_{\varphi\psi}$ over diffracting grains along the measurement direction **n**.

Using Eq. 11, we simulated uniaxial tensile tests and plotted the evolution $\varepsilon_{\varphi\psi}$-vs.-$\sin^2\psi$ diagrams for different polycrystals with cubic or hexagonal symmetry. An isotropic crystallographic texture has been used to highlight only the influence of the morphologic texture.

The morphologic texture is incorporated in the model by considering ellipsoidal inclusions with their principal axes aligned along common directions in the specimen frame of reference. The shape of the crystallites has been described by a shape parameter denoted η, which is defined as the ratio of the principal axis of the ellipsoid (a_3) and the secondary axes (a_1 or a_2) of the ellipsoid (see Fig. 1).

$$\eta = \frac{a_3}{a_1} = \frac{a_3}{a_2} \tag{18}$$

Shape parameters used to describe the morphologic textures investigated in this work are given below (by considering $a_1 = a_2 = 1$):

- $\eta = 1$ for spherical grains
- $\eta = 100$ for fiber shape
- $\eta = 0.01$ for disc shape

These shape parameters (for fibers and discs) have been chosen to take into account an extreme morphologic texture.

The mechanical response of a transversely isotropic material differs depending on the morphologic orientation of the grains. To account for the influence of the morphologic orientation of the grains, we simulated an uniaxial tensile test with a macroscopic stress $\sigma_{11}^{I} = 100$ MPa by varying the morphologic orientation of the grains in the sample (see Fig. 4). For each considered morphology, three different simulations are then performed:

- first, when grain principal axes (a_3) are aligned preferentially along the loading direction ($a_3 // S_1$).
- Secondly, when the (a_1) axes of the grains are aligned preferentially along the loading direction and (a_2) perpendicular to the specimen surface S ($a_1 // S_1$, $a_2 \perp S$).
- Finally, when the (a_1) axes of the grains are aligned preferentially along the loading direction and (a_3) perpendicular to the specimen surface S ($a_1 // S_1$, $a_3 \perp S$); this latter corresponds to the case of thin films with columnar grains, when a fiber or disc texture is considered.

In the remainder of the paper and for more clarity, the cases ($a_3 // S_1$), ($a_1 // S_1$, $a_2 \perp S$) and ($a_1 // S_1$, $a_3 \perp S$) have been denoted C1, C2 and C3, respectively.

Several lattice-planes commonly used to perform lattice strains measurements in XRD [8, 38–43] and ND [44–48] have been investigated. In order to compare the influence of the morphologic texture on stress analysis by XRD and ND methods, we have chosen to present only the results obtained for (*hkl*) planes in common to these two diffraction techniques (see Table 2).

The elastic strains $\varepsilon_{\varphi\psi}$ have been plotted as a function of $\sin^2\psi$ in Fig. 5 for (200) and (220) planes of the gamma-iron and (00.4) and (10.4) planes of the zinc, by taking into account the different morphologic orientations of the grains defined in Fig. 4. For the sake of clarity, only the average strains were plotted. We note that the anisotropy introduced by the morphologic texture has greatly changed the $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ distributions for some (*hkl*) planes. More or less oscillations were observed, depending on the lattice plane analysed. For a given extreme grain shape (fiber or disc), the $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagram deviates from the one obtained for a non-textured material composed of spherical crystallites. The linearity of the $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ curves is preserved for the case (a_1 // S_1, $a_2 \perp S$) but their slopes are more or less different from that obtained on a macroscopically isotropic polycrystal according to the morphologic texture considered (strong deviations have been observed for the disc texture). For the two others cases of loading, this linearity is no longer preserved.

Different $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ distributions have been observed according to the grains shape, their orientation in the specimen, the (*hkl*) lattice plane and the polycrystal investigated (i.e. whether gamma-iron or zinc is studied). As indicated in the previous section, experimental determinations of an unknown state of stress (residual or internal stresses) are usually performed with these curves and XECs $\frac{1}{2}S_2(hkl)$ and $S_1(hkl)$ values of the specimen, using Eq. 14, instead of the stress factors [18–22]. Due to the influence of the morphologic texture on the $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams, their interpretation in terms of macroscopic stresses will, therefore, lead to a state of stress more or less far from the real stress in the material. Because some diagrams are not linear, the stress determined by XRD and ND methods can be different. To avoid all these deviations, a proper selection of reflections less sensitive to the morphologic texture is crucial, hence the interest to study the influence of the morphologic texture on the different planes used in diffraction technics.

The stresses are calculated using an elliptical regression $A\sin^2\psi\ B\sin 2\psi + C$ (Eq. 14) curves of each $\varepsilon_{\varphi\psi}$-vs.-$\sin^2\psi$ diagrams obtained. Due to the uniaxial state of stress considered (absence of shear stress), *B* coefficients obtained are practically zero and regressions are linear rather than elliptical and have the form of Eq. 17. The stress component $\sigma^I_{11,determined}$ determined from these regressions is then compared to the real stress $\sigma^I_{11,expected}$ in the material in terms of relative deviation:

$$\Delta\sigma^I_{11} = \frac{\left|\sigma^I_{11,determined} - \sigma^I_{11,expected}\right|}{\sigma^I_{11,expected}} \times 100 \qquad (19)$$

Furthermore, the calculated deviations are a helpful tool to quantify the influence of the morphologic texture on the mechanical properties at an intermediate scale corresponding to the diffracting volume. The results obtained for the gamma-iron (γ-Fe) and the zinc (Zn) have been presented in Table 2. A maximal relative difference of 27.2 and 38.1 % has been observed for the gamma-iron and the zinc, respectively. However, one can observe that some planes are less influenced by the morphologic texture depending on the microstructure (fiber or disc) and their orientation (($a_3 // S_1$), ($a_1 // S_1$, $a_2 \perp S$) and ($a_1 // S_1$, $a_3 \perp S$)); it is the case for example for (10.0), (00.4), (11.0), (20.1) and (30.2) planes of the zinc with fiber texture when ($a_3 // S_1$).

For example, analyzing zirconium (or zirconium alloy) sample by XRD, experiments were carried out on the lattice plane (10.4) ($2\theta \approx 156°$) using a Cr radiation [39]. If a disc texture with a morphologic orientation ($a_3 // S_1$) exists in the polycrystal, a relative deviation of 27 % is observed on the determined stress. In this case, it would be better to use the (30.2) lattice plane with Cu radiation which will give only 6 % of relative deviation.

To show the relevance of the model, we compare our calculations to experimental data from the literature. Because the main interest of this contribution is to highlight the influence of the morphologic texture, we choose to compare our calculations to experimental data obtained by Faurie et al. [49] on non-textured (i.e crystallography texture does not occur) gold films. The measurements were performed using synchrotron X-ray diffraction combined with *in situ* tensile tests. For each applied (uniaxial) load to the dog-bone specimen (film + substrate), the authors calculated the resulting biaxial stress in the non-textured gold films; these values can be found in [49]. The measurements were performed for the longitudinal direction ($\varphi = 0°$) and for 8 different ψ values (ranging from 0° to 66°).

From the equation 11, we simulated $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams for (222) and (420) planes, which are then compared to experimental data [49]. 20000 grains with random crystallographic orientations are used to describe the texture-free state of the gold films. Due to the small thickness of the films (500 ± 10 nm), the morphologic texture of the crystallites has been described by disc-shaped grains which axis are perpendicular to the specimen surface (C3 case in Fig. 4). The single-crystal elastic constants used are c_{11} = 190 GPa, c_{12} = 161 GPa and c_{44} = 42.3 GPa [50]. Fig. 6 shows $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ curves for (222) and (420) planes for the 3 biaxial stress states (denoted T_1, T_2 and T_3) applied to the specimen, computed assuming either an isotropic morphologic texture (spherical grains) or a disc grain morphology. A very satisfactory fitting of measured data is obtained considering the disc texture rather than spherical grains. The influence of the morphologic texture is more noticeable on the $\sin^2\psi$ plots for the 222 reflection, especially when the applied load is important. A very good agreement between the experiment and the model is observed.

4. Influence of crystallographic texture on the diffraction stress analysis

The presence of a crystallographic texture in polycrystalline materials is not an exception: any polycrystalline material has necessarily a crystallographic texture either weak or strong. The evaluation of residual stresses in crystallographically textured materials will not be discussed here. A detailed description can be found in [26, 28, 32, 51]. The aim of this section is to evaluate the crystallographic texture effect in the stress analysis by diffraction technics in order to make a comparison with the morphologic texture effect.

A rolled texture simulated by a Taylor viscoplastic model [52] with a final plastic strain of 80 % is used to define the crystallographic texture of polycrystals with cubic structure (face centered cubic or body centered cubic structures). For polycrystals with hexagonal structure, we used an experimental ODF of zircaloy-4 plate cold-rolled with a total strain rate of 47 % [53]. Some pole figures of these crystallographic textures are shown in Fig. 7.

Texture can be quantified in the model by introducing the ODF specifying the volume fraction of crystallites having a given orientation $\mathbf{\Omega}(\varphi_1,\phi,\varphi_2)$. Fig. 8 shows $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams of the (200) and (220) lattice planes of the gamma-iron, (00.4) and (10.4) of the zinc, in the case of crystallographic texture (spherical grains are considered). The crystallographic texture leads to non-linear distributions of $\varepsilon_{\varphi\psi}$-*vs*.-$\sin^2\psi$ curves, except for (200) and (00.4) planes. No oscillation occurred on (222) plane $\varepsilon_{\varphi\psi}$-vs.-$\sin^2\psi$ plots (not shown here) in spite of the crystallographic texture. This confirms the results of [51] who verified experimentally that *hhh* and *h00* reflections could be used without knowledge of the crystallographic texture because their XECs are independent of φ and ψ angles. The missing points in the vertical bars or rows of points in this figure, comparatively to Fig. 3, are due to the suppression of some orientations $\mathbf{\Omega}(\varphi_1,\phi,\varphi_2)$ of the diffracting grains and their reorientations in the preferential directions.

Commonly, for crystallographically textured materials, XECs depend on the measurement direction, but the values calculated from isotropic materials are often used, for the sake of simplicity, in stress analysis by diffraction methods. As in the previous case, a study has been done using XECs calculated from spherical grain (isotropic texture). Relative differences using Eq. (19) on determined stresses for the gamma-iron (γ-Fe) and the zinc (Zn) have been presented in Table 3. Only a maximal relative difference of 13.3 % and 11.9 % has been observed for the gamma-iron and the zinc, respectively, although these crystallographic textures are strongly marked.

5. Combined effects of crystallographic and morphologic textures on stresses analysis by diffraction

The mechanical behaviour of a polycrystalline material depends not only on its crystallographic texture but also on its morphologic texture. We have shown that each of these two forms of textures can greatly influence the results of stress analysis by XRD and ND technics; a stronger influence in the case of the morphologic texture has been observed. Usually, in a polycrystalline material, these two types of textures are susceptible to occur simultaneously, influencing the multi-scale mechanical properties and thus the results of stress analysis by diffraction methods. It is therefore necessary to focus on the combined effects of these two types of textures on the stress analysis by diffraction. The morphologic texture (fibers and discs) and crystallographic one mentioned in the previous paragraphs are used to evaluate the combined effects of crystallographic and morphologic textures in the stress analysis.

The $\varepsilon_{\varphi\psi}$ strains have been plotted as a function of $\sin^2\psi$ in Fig. 9 for (200) and (220) planes of the gamma-iron and (00.4) and (10.4) planes of the zinc. For each considered morphology, three different simulations have been achieved:

- first, when grain principal axes (a_3) are aligned preferentially along the loading direction (a_3 // S_1 // RD); the loading direction (S_1 axis) corresponds to the rolling direction (RD) in the case of the fiber texture and to the transverse direction (TD) in the case of the disc texture,
- secondly, when the (a_1) axes of the grains are aligned preferentially along the loading direction and (a_2) perpendicular to the surface of the specimen (a_1 // S_1 // TD, $a_2 \perp S$),
- and finally, when the (a_1) axes of the grains are aligned preferentially along the loading direction and (a_3) perpendicular to the sample surface (a_1 // S_1 // TD, $a_3 \perp S$).

For the two last cases, the loading direction corresponds to RD for the disc texture and TD for the fiber texture.

We note that these curves differ from those obtained using only the effects induced by either a morphologic (Fig. 5) or a crystallographic texture (Fig. 8). By observing the evolution of these curves, we can deduce that the interpretation of these latters will lead, obviously, to different values of stresses (more or less different from the real stresses in the material).

Table 4 gives relative deviations on determined stresses by diffraction, due to the combined effects of crystallographic and morphologic textures.

The relative deviations obtained are greater than those resulting from morphologic and crystallographic textures, separately taken into account. A maximal relative difference of 36.6 % is observed for the gamma-iron and 44.4 % for the zinc.

To show the ability of the model to take into account the combined effects of crystallographic and morphologic textures in the stress analysis by diffraction, our calculations have been compared to experimental data published by a research group, on the basis of mechanical tests measurements. We compare our calculations to experimental data obtained by Renault et al. [54] on (111)-textured gold films. X-ray diffraction measurements were performed on a dog-bone specimen (film + substrate), using a four-circle goniometer. The specimen was subjected to four uniaxial increasing loading states $T_1^{'}$ = 0.7 MPa, $T_2^{'}$ = 1.3 MPa, $T_3^{'}$ = 1.8 MPa and $T_4^{'}$ = 2.5 MPa. Three different (*hkl*) planes were analysed: (222) at ψ = 0°, (400) at ψ = 54.74°, (311) at ψ = 29.5° and 58.5°. The measurements were performed in the longitudinal (S_1) and transversal (S_2) directions. Using a least-squares problem, the authors determined the elastic single-crystal compliances of the textured anisotropic gold film. The compliances found were slightly different from the corresponding bulk material ones.

We have simulated $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ curves for the (*hkl*) planes experienced by [54], using the single-crystal elastic constants given by [50]. The morphologic texture of the crystallites has been described by disc-shaped grains which axis are perpendicular to the specimen surface (C3 case in Fig. 4), due to the small thickness of the films (260 nm). A (111) fiber-texture has been simulated with a dispersion of 8° around the S_3 axis, generally observed in the thin films [55]. 20000 orientations have been selected to describe the crystallographic texture of the thin films. Fig. 10a shows the corresponding simulated (111) pole figure. For each applied load, the biaxial stresses resulting in the gold film have been calculated and the corresponding values are given in Table 5. Fig. 10b shows lattice strains $\varepsilon_{\varphi\psi}$ plotted versus $\sin^2\psi$ in the longitudinal direction (φ = 0°) and the transversal one (φ = 90°), for the four declination angles ψ. Once again, a good agreement between experiment and simulation can be observed in Fig.10b. It can be conclude that the self-consistent model can describe the measured $\sin^2\psi$ plots of the films analysed.

6. Discussion

From the above sections, one can notice that all planes would not provide the same stress values: some planes are less sensitive to the effects of texture (crystallographic, morphologic or combined effects of both textures); some are strongly influenced by the effects of texture. We have shown that the morphologic texture, often neglected in the context of achieving stress analysis by XRD and ND technics, is the main cause of the relative discrepancies obtained between the calculated and the applied macroscopic stress values. The morphologic texture denotes not only the shape of the grains, but also their orientation relative to the loading or residual stress direction (as showed in Fig. 4).

Traditionally, in stress analysis, a macroscopically elastically isotropic specimen is considered. In this case, the only way to avoid or to minimize the effects of morphologic texture in stress analysis is to make a good choice of (*hkl*) planes when performing lattice strain measurements. First, note that the morphologic texture does not have the same effects on all the polycrystalline materials, as observed for the gamma-iron and the zinc. Studies presented in this paper were conducted on several materials; we observed that morphologic texture effects depend on the elastic anisotropy coefficient A_c of the single crystal of the material ($A_c = 2c_{44}/(c_{11} - c_{12})$ for polycrystals with cubic structure and $(c_{11} + c_{12} - c_{33})/c_{13}$ for polycrystals with hexagonal structure [25]). An elastic anisotropy coefficient of the single crystal close to 1, minimizes the effects of morphologic texture in the stress analysis by diffraction (the results obtained for aluminum, beryllium, titanium confirm this latter). The influence of the morphologic texture increases as the elastic anisotropy coefficient A_c deviates from 1. It is the case for example of gamma-iron, zinc or copper. Thus, any (*hkl*) plane can be used without knowledge of the morphologic texture, when the elastic anisotropy coefficient of the single crystal of the material is close to 1. On the other hand, when A_c is more important (about 2 or more), some (*hkl*) planes are best suited for the stress analysis by XRD and ND technics and some are to be avoided. For example, analyzing aluminium ($A_c \approx$ 1.22) [38] by XRD, experiments are carried out on the lattice plane (222) ($2\theta \approx$ 156.71°) using a Cr radiation [8]. If a disc texture with a morphologic orientation ($a_3 // S_1$) and a marked crystallographic texture exists in the polycrystal, a low relative deviation (5.6 %) would be observed on the determined stress. For the others planes, relative deviation observed would not exceed 5 %. In this case, any (*hkl*) plane could be used. In gamma-iron ($A_c \approx$ 3.34), XRD experiments are carried out on the lattice planes (311) and (222) ($2\theta \approx$ 126.83° and 138.15° respectively) using a Fe radiation (Hauk, 1997). If a crystallographic texture exists, a relative difference of 36.6 % is observed for the stresses determined on the (222) reflection whereas the discrepancy reduces to 11.7 % for the (311) plane in the C3 case of the disc texture. On the other hand, in the C1 case of the fiber texture, only 0.3 % of relative difference is observed using (222) plane and 14.7 % using (311) plane.

According to the previous results, we propose a selection criterion (Table 6) to choose the (*hkl*) planes for stress analysis by diffraction, to minimize the effects of morphologic texture or the combined effects of crystallographic and morphologic textures. Table 6 concerns materials with an elastic anisotropy coefficient A_c about 2 or more. The appropriate (*hkl*) planes in this Table take into account the morphologic and crystallographic textures indicated in Fig. 4 and Fig. 7, respectively.

The maximal relative difference on the determined stresses, below which an (*hkl*) plane is considered favourable is 10 %. This value has been chosen arbitrarily. If the relative differences are between 10 and 20 %, the choice of the corresponding lattice planes should be avoided if possible. (*hkl*) planes with a relative difference up to 20 % should be strictly avoided. We note that each (*hkl*) plane can be favourable or not, depending on the morphologic texture of the polycristal, except (844) plane which is an appropriate choice for stress analysis whatever the texture.

7. Conclusion

The morphologic texture influence on macroscopic stress determination, by diffraction methods in polycrystals having cubic or hexagonal symmetries, were investigated by Eshelby-Kröner self-consistent calculations. A stronger influence of morphologic texture in terms of stresses was observed. These effects of morphologic texture depend on the type of the grain shape considered (fiber or disc), the direction of the applied stress, the grains morphologic orientation in the sample, the inclination angles ψ used and the single crystal elastic anisotropy. The predicted mechanical behaviour is compared with published experimental results and a good agreement between theory and experiment was found. Numerical results obtained at the different scales of the material show the relevance of this approach for polycrystalline materials and validate the scale transition method used. If the single crystal of the material is almost elastically isotropic, any (*hkl*) plane can be used without knowledge of the morphologic texture. In this case, the maximal relative discrepancy on determined stresses observed is about 10%. For materials exhibiting strongly anisotropic elastic properties at mesoscopic level coupled with extreme morphologic texture of fiber or disc and a crystallographic one (either weak or strong), it was found that the measured diffraction strain is strongly dependent of the grain shape texture causing the observed non-linearities in the $\varepsilon_{\varphi\psi}$-vs.-$\sin^2\psi$ plots. In this case, the use of diffraction (X-ray) elastic constants causes errors (up to 44.4 %) in the stress analysis. To circumvent this problem, a selection criterion was proposed to choose (*hkl*) planes favourable to stress analysis by diffraction technics. By using favourable (*hkl*) planes, XECs can be used instead of the stress factors which evaluation is more complex than XECs.

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Table 1 XECs $1/2S_2$ (10^{-6} MPa^{-1}) as a function of the diffracting planes (hkl), calculated using Eshelby-Kröner self-consistent model.

Table 2 Relative deviation (in %) on determined stresses by diffraction methods, due to the effects of morphologic texture; C1, C2 and C3 correspond to (a_3 // S_1), (a_1 // S_1, $a_2 \perp S$) and (a_1 // S_1, $a_3 \perp S$) cases, respectively. Relative differences exceeding 10 % are highlighted in bold.

Table 3 Relative deviation (in %) on determined stresses by diffraction methods, due to the effects of crystallographic texture, along the rolling direction (RD) and the transverse one (TD). Relative differences exceeding 10 % are highlighted in bold.

Table 4 Relative deviation on determined stresses by diffraction technics, due to the combined effects of crystallographic and morphologic textures; C1, C2 and C3 correspond to (a_3 // S_1 // RD), (a_1 // S_1 // TD, $a_2 \perp S$) and (a_1 // S_1 // TD, $a_3 \perp S$) cases, respectively. Relative deviation exceeding 20 % are highlighted in bold.

Table 5 Values of the applied forces and resulting applied stresses in the (111)-textured gold films.

Table 6 Recommendations on the choice of the lattice-plane in stresses analysis by diffraction methods according to the morphologic texture of the single-phase polycristal with A_c about 2 or more. C1, C2 and C3 correspond to (a_3 // S_1 // RD), (a_1 // S_1 // TD, $a_2 \perp S$) and (a_1 // S_1 // TD, $a_3 \perp S$) cases, respectively; according to the relative deviation on determined stresses, some (*hkl*) planes should be: (+) favourable for stresses analysis by diffraction methods below 10 %, (-) avoided, if possible, between 10 and 20 % and (×) strictly avoided, above 20 %.

Fig. 1 Definition of the geometry of the extreme morphologic textures studied.

Fig. 2 Geometry of the diffraction: definition of the rotation angle φ of the sample around the sample surface normal (3) and the inclination angle ψ of the sample surface normal with respect to the diffraction vector **n** (aligned along the L_3 axis); (S_1, S_2, S_3) is the sample reference frame and (L_1, L_2, L_3) the laboratory reference frame.

Fig. 3 $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams for non-textured isotropic materials. (●) second order lattice strain of each crystallite participating in the diffracting volume; (····◆···) diffracting volume average lattice strain.

Fig. 4 Different morphologic orientations of the grains in the samples.

Fig. 5 $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams for morphologically textured materials, diffracting volume average lattice strain: (—■—) loading direction parallel to (a_3) grain axes (a_3 // S_1); (—▲—) loading direction parallel to (a_1) grain axes and (a_2) perpendicular to the surface of the specimen (a_1 // S_1, $a_2 \perp S$); (—●—) loading direction parallel to (a_1) grain axes and (a_3) perpendicular to the surface of the specimen (a_1 // S_1, $a_3 \perp S$); (—◆—) non-textured isotropic case (spherical grains). (for colored figure, reader is invited to see the article web version).

Fig. 6 $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ curves for (222) and (420) planes for the 3 biaxial stress states (T_1, T_2 and T_3), using an isotropic morphologic texture (spherical grains) and a disc texture. Continuous lines represent the theoretical strains obtained from the Eshelby-Kröner model; the symbols (◆ : T_1, ■: T_2, ▲: T_3) represent the experimental strains [49].

Fig. 7 Pole figures of crystallographic textures used to simulate the elastic behaviour of materials with cubic (a) and hexagonal (b) crystal system. RD: rolling direction; TD: transverse direction.

Fig. 8 $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams for crystallographically textured materials. (●) second order lattice strain of each diffracting crystallite for the considered (*hkl*) plane; (····◆···) diffracting volume average lattice strain; (——) non-textured isotropic case.

Fig. 9 Combined effects of crystallographic and morphologic textures on $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ diagrams, diffracting volume average lattice strain: (—■—) loading direction parallel to (a_3) grain axes and RD (a_3 // S_1); (—▲—) loading direction parallel to (a_1) grain axes and (a_2) perpendicular to the surface of the specimen (a_1 // S_1, $a_2 \perp S$); (—●—) loading direction parallel to (a_1) grain axes and (a_3) perpendicular to the surface of the specimen (a_1 // S_1, $a_3 \perp S$); (—◆—) non-textured isotropic case (spherical grains); for (a_1 // S_1, $a_2 \perp S$) and (a_1 // S_1, $a_3 \perp S$) cases, the loading direction corresponds to RD for disc texture and TD for fiber texture.

Fig. 10 (a) Simulated (111) pole of the (111)-textured gold films with a dispersion of 8° around the S3 axis; (b) $\varepsilon_{\varphi\psi}$-*vs.*-$\sin^2\psi$ curves for the 4 loading states; using an isotropic morphologic texture (spherical grains) and a disc texture; open symbols (- ⊟ -: $T_1^{'}$, - △ -: $T_2^{'}$, - ◇ -: $T_3^{'}$, - ⊖ -: $T_4^{'}$) represent the theoretical strains obtained from the Eshelby-Kröner model; full symbols (—■—: $T_1^{'}$, —▲—: $T_2^{'}$, —◆—: $T_3^{'}$, —●—: $T_4^{'}$) represent the experimental strains [54].