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A generic method for modeling the behavior of anisotropic metallic materials: Application to recrystallized zirconium alloys

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Abstract

A simplified polycrystalline model (the so-called RL model) is proposed to simulate the anisotropic viscoplastic behavior of metallic materials. A generic method is presented that makes it possible to build a simplified anisotropic material texture, based on the principal features of the pole figures. The method is applied to a recrystallized zirconium alloy, used as clad material in the fuel rods of nuclear power plants. An important database consisting in mechanical tests performed on Zircaloy tubes is collected. Only a small number of tests (pure tension, pure shear) are used to identify the material parameters, and the texture parameters. It is shown that six crystallographic orientations (6 "grains") are sufficient to describe the large anisotropy of such hcp alloy. The identified crystallographic orientations match the experimental pole figures of the material, not used in the identification procedure. Special attention is paid to the predictive ability of the model, i.e., its ability to simulate correctly experimental tests not belonging to the identification database. These predictive results are good, thanks to an identification procedure that enables to consider the contribution of each slip system in each crystallographic orientation.

Keywords: Anisotropic material; Constitutive behaviour; Crystal plasticity; Polycrystalline material; Zirconium alloys

1. Introduction

Since the pioneering work of Hill (1950), several efforts have been made to improve the description of initial plastic anisotropy according to macroscopic constitutive equations (see for instance, Gotoh, 1977; Barlat et al., 1991; Karafillis and Boyce, 1993; Bron and Besson, 2004; Nemat-Nasser, 2004). Nevertheless, these macroscopic models generally fail to accurately represent non-proportional and cyclic loadings (Cailletaud and Pilvin, 1994). Especially, the simulation and prediction of the yield surface distorsion remain difficult to achieve with classical phenomenological models, and more or less complicated improvements of these models do not give total satisfaction (Vincent et al., 2002; Kuroda and Tvergaard, 2001).

Polycrystalline models generally give a good description of the plastic anisotropy and yield

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surface distorsion, because they are based intrinsically on slip lattice as well as texture information (Cailletaud, 1992; Pilvin, 1990; Calloch, 1997). Nevertheless, their main disadvantage is the large computation times needed for parameter identification and finite element calculations. Indeed, these models are built in such a way that the number of internal variables to compute may be a thousand times larger than the number of internal variables using a phenomenological model. Thus one understands the relatively rare use of polycrystalline models in industrial calculations.

In the field of nuclear industry, important work has been done on the viscoplastic behavior of zirconium alloys, using phenomenological models as well as polycrystalline approaches, both combined to experimental multi-axial tests performed on tubes. These multi-axial tests (pure tension, biaxial tension, tension–torsion) are necessary to investigate the material response to the complex loadings that are applied to the nuclear fuel rods in Pressurized Water Reactors. It can be seen that an accurate description of the anisotropy and irradiation effects requires quite a complex set of equations in phenomenological approaches (Robinet, 1995; Schaeffler, 1997; Richard et al., 2003) while the multi-scale approach allows much simpler developments (Lebensohn and Tomé, 1993; Geyer, 1999; Onimus, 2003). Nevertheless, none of these models is used at present time in really industrial finite element calculations because of their complexity or too large CPU time.

In order to combine the good predictive ability of polycrystalline approaches and the moderate CPU time necessary to conduct safety analyses for the nuclear industry, we propose in the present paper a simplified polycrystalline model (the so-called RL model – Rousselier and Leclercq, 2006) to simulate the anisotropic viscoplastic behavior of metallic materials. A generic method is presented that makes it possible to build a simplified anisotropic material texture, based on the principal features of the pole figures. The method is applied to recrystallized zirconium alloys. The model aims at representing the mechanical behavior of polycrystals with a minimum number (between 5 and 10) of crystalline orientations (“grains”), and considers only six slip systems by grain for describing the inelastic strain tensor, whatever the crystallographic lattice of the material under study is. It must be very clear that our goal is not to represent accurately the material texture, but only its mechanical effect on the response of a structure to a mechanical loading. Nevertheless, we show in the following that our choice of the crystallographic orientations is closely related to the real material texture, and moreover that it can be identified thanks to an optimization algorithm by comparison with the results of experimental tests.

We must emphasize that the idea of improving the micro-macro models to make them useful for element computations has already been developed by Gittus and Zarka (1986), Gittus et al. (1986) and Zarka and Navidi (2005).

In the next section, we recall the major features of the simplified viscoplastic RL-polycrystalline model. In Section 3, we show how the model has been applied to the simulation of the anisotropic behavior of a recrystallized zirconium alloy. Particular attention is paid to the description of the parameter identification of the model using several multi-axial tests. An example of finite element calculation performed on a tube is presented in Section 4. Concluding remarks are given in the last section of this paper.

2. The simplified viscoplastic RL-polycrystalline model

The model is presented in the case of small deformations and small rotations. We want to emphasize that the RL model does not depart from classical polycrystalline models. Consequently, all existing and future theoretical and software developments apply easily to the model, with regard for example to finite deformations, rotation of crystallographic orientations, localization self-consistent models, or slip systems constitutive equations.

Let $\underline{n}_s$ be the normal vector of a slip plane and $\underline{l}_s$ the unit slip direction vector. The orientation tensor of the slip system number s is defined as

$$\underline{\underline{m}}_s = (\underline{n}_s \otimes \underline{l}_s + \underline{l}_s \otimes \underline{n}_s)/2 \tag{1}$$

We consider only six universal slip systems corresponding to shear and extension strain rates in the local frame $x_1x_2x_3$ of a given crystallographic orientation (Fig. 1):

$$\underline{n}_1 = [1\ \ 0\ \ 0], \quad \underline{n}_2 = [0\ \ 1\ \ 0], \quad \underline{n}_3 = [0\ \ 0\ \ 1]$$
$$\underline{l}_1 = [0\ \ 1\ \ 0], \quad \underline{l}_2 = [0\ \ 0\ \ 1], \quad \underline{l}_3 = [1\ \ 0\ \ 0]$$

$$\underline{\underline{m}}_1 = \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \underline{\underline{m}}_2 = \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$
$$\underline{\underline{m}}_3 = \frac{1}{2}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$