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Measurement and prediction of residual stresses and crystallographic texture development in rolled Zircaloy-4 plates: X-ray diffraction and the self-consistent model

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Abstract

Complementary methods were used to analyse residual stresses and texture evolution in Zircaloy-4 sheets which had undergone cold-rolling deformation: X-ray diffraction and the self-consistent model. A modified elastoplastic self-consistent model, adapted to large deformation, was used to simulate the experimental results and showed close agreement with the experimental data. A new formulation of crystal plasticity is proposed. The influence and the role of elastoplastic anisotropy were also studied and explained in this work. Good agreement was found between experimental and predicted crystallographic textures. The contribution and the magnitude of the first- and second-order residual stresses were correctly evaluated using information from the model. Comparison between the X-ray diffraction results and the simulations confirms that prismatic slip is the main active deformation mode in this alloy under large strain.

Keywords: X-ray diffraction; Texture; Residual stresses; Micromechanical modelling

1. Introduction

Zirconium alloys are widely used in the nuclear industry because they exhibit a high resistance to corrosion, a good thermal conductivity and a low absorption cross-section for thermal neutrons. They have a hexagonal close-packed structure at room temperature. These alloys present highly anisotropic plastic properties at mesoscopic (grain) and macroscopic levels with various active deformation modes. These properties and the crystallographic texture explain the appearance and development of important residual stresses when an elastoplastic deformation is introduced. These stresses depend on initial and induced crystallographic textures, and are termed intergranular or second-order stresses. They appear experimentally after unloading as tensile or compressive residual elastic strains.

The engineering consequences of second-order stresses with strong texture may be severe [1]. Therefore, metal-forming processes optimization such as rolling requires knowledge of the evolution of the material's anisotropic elastoplastic behaviour during the deformation operations. The modelling of the plastic deformation of metallic polycrystals can be carried out by deductive methods based on strain mechanisms and scale transition methods like those of Taylor [2] or self-consistent (SC) models [3–8]. Micromechanical modelling seems to be particularly well suited to describe the material evolution during deformation processes. 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 morphological texture. The crystalline lattice rotations, which lead to the crystallographic texture of the polycrystal, are calculated for each grain. Generally, each grain is considered as a uni-

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form entity with uniform stress and strain fields. The intracrystalline behaviour of grains is built from internal variables which describe the rate of plastic glide on active slip systems according to Schmid's law.

Polycrystal models are typically evaluated by their ability to simulate the mechanical behaviour. For large deformations (>20% strain), model predictions are readily compared with textures determined experimentally by X-ray or neutron diffraction. Various attempts to explain zirconium alloys textures were performed [9,10], in particular with an SC viscoplastic approach [11–13].

In the case of small deformations, texture development is minimal and cannot serve as a way of assessing the model predictions. However, the model can be evaluated on a much more specific micromechanical level using the technique of lattice strain characterization by diffraction techniques. Diffraction techniques provide the possibility of determining the elastic lattice strain in selected grain subsets within the polycrystal as a function of the applied load. Such results can be compared directly with model predictions of volume-average elastic lattice strains in selected diffracting grain subsets. In this case, the different material parameters (hardening matrix, critical resolved shear stresses) can be found by fitting the macroscopic loading curves and then validating them with diffraction results. Such approaches were used with success to explain the plastic behaviour of zirconium alloys like Zircaloy-2 [14,15] or zirconium-α [16–18].

Hexagonal materials are characterized by a wide variety of possible deformation systems. It is necessary to know both the texture and the deformation mechanism to be able to model these mechanical properties. This requires, in particular, a proper knowledge of the deformation mechanisms with their corresponding critical resolved shear stresses (CRSS). Only few data are available for CRSS in the literature. Moreover, the CRSS generally depend significantly on the contents of alloying elements. In spite of this very basic knowledge of these data, many authors have tried to model the mechanical properties of hexagonal materials after large deformation. In these cases, the approach consists in finding the set of material parameters offering the best agreement with the crystallographic texture by applying a polycrystalline model.

In the present work, a different approach is proposed to validate the accuracy and relevance of a theoretical model for hexagonal material in a large deformation framework. To the knowledge of the present authors, characterization of both texture and residual stresses by diffraction have never been used simultaneously to evaluate polycrystal models for non-cubic material.

The purpose of this study is to combine experimental observations (X-ray diffraction) with the predictions of an elastoplastic self-consistent (EPSC) model in order to obtain more information about the different factors responsible for the appearance of residual second-order stresses. This comparison allows a better understanding and interpretation of diffraction and mechanical results. Diffraction methods are helpful techniques to characterize the mechanical state of polycrystalline materials at the mesoscopic level. Characterization is performed from the elastic strains measurement and the subsequent calculation of the stress state by means of mechanic equations. The capacity to measure intergranular strains provides an experimental tool for understanding how intergranular strains are generated. Diffraction data offer a rigorous test for the models at a microscopic level [6,19–21]. The comparison with experimental texture and residual stresses should allow a more accurate interpretation of scale transition approach like the EPSC model.

In this work, a complete study concerning the development and evolution of residual stresses and texture introduced by cold-rolling tests in polycrystalline Zircaloy-4 (Zy-4) sheets was made. An EPSC model was used to simulate the mechanical response of samples tested along the initial rolling direction of the sheet. A modification concerning the selection of active slip systems was made for the present model and a new formulation of the crystal plasticity was proposed. This algorithm is much faster and resolves the problem of ambiguous selection of slip systems. The theoretical stresses are compared with the experimental results obtained by X-ray diffraction. The results predicted by the SC model are discussed. In particular, twinning mode is treated as a directional deformation system, and the reorientation by slip and twinning is taken into account in our calculations. In hexagonal alloys, like those of 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, as well as the first-order (macroscopic) stresses, has also been performed.

2. Experiments

2.1. Samples

In the present study, a cold-rolled Zircaloy-4 (Zy-4) sheet is considered. The aggregate exhibits equiaxed grains with a mean size of 25 μm. To analyse the mechanical behaviour of the material at large deformation, two samples (the dimensions were 92 mm × 16 mm × 2 mm) were cut along the rolling direction (RD) of the sheet. The specimens were submitted to cold-rolling tests at room temperature along the original RD of the sheet. The total strains are 30.5% and 47% for the first and the second tests. The chemical composition is (wt.%; balance = Zr): Sn (1.4), Fe (0.21), Cr (0.09) and O (0.12).

2.2. Texture analysis

X-ray diffraction analysis was performed with a four circles XRD3003PTS SEIFERT goniometer. Kα copper radiation was used. The X-ray beam output collimator had a