Texture Variations and Cyclic Softening Mechanisms on ZRY-4 at Room Temperature. Part II: Texture Evolution and Simulations

R. E. Bolmaro¹, J.W. Signorelli¹, H.-G. Brokmeier², A. F. Armas¹, S. Hereñú¹ and I. Alvarez-Armas¹

¹ Instituto de Física Rosario, CONICET-Universidad Nacional de Rosario, Bv. 27 de Febrero 210 Bis, 2000.
e-mail: bolmaro@ifir.edu.ar, signortel@ifir.edu.ar, armas@ifir.edu.ar, erenu@ifir.edu.ar, alvarez@ifir.edu.ar;
² Institute of Material Engineering, GKSS-Research Center, Max-Planckstr., D-21502 Geesthacht, Germany
e-mail: Heinz-Guenter.Brokmeier@gkss.de

RESUMEN

La Parte I del presente trabajo muestra resultados de ensayos de fatiga y los correspondientes análisis, todos prácticamente probatorios de que la hipótesis de reorientación de los sistemas de deslizamiento prismático, como modo de explicar el ablandamiento cíclico, debería desecharse. La presente Parte II del trabajo muestra mediciones de texturas en otra serie de muestras sometidas a ensayos de fatiga. Las texturas fueron medidas por medio de rayos X y neutrones y son analizadas por métodos habituales de cálculos de Funciones de Distribución de Orientaciones Cristalinas. Las texturas son utilizadas a su vez como datos de partida para modelos de simulación que permiten calcular la evolución de la tensión aplicada en función de la textura y a lo largo de un ciclo completo de carga. Los resultados obtenidos muestran que la hipótesis de reorientación de sistemas de deslizamiento debería desecharse en beneficio de modelos más tradicionales de interacción dislocaciones-defectos puntuales.

Palabras clave: Fatiga de bajo número de ciclos, difracción de rayos x, textura, modelos micro mecánicos, ablandamiento cíclico.

ABSTRACT

Part I of the current paper has shown fatigue test results and its corresponding analysis. All of them practically reject the hypothesis of crystal reorientation and cyclic softening being consequence of prismatic slip system rotation. The present Part II of the paper shows texture measurements in another series of cyclic deformed samples. The textures were measured by both x-rays and neutron diffraction and were analyzed by Crystal Orientation Distribution Function analysis. The textures were used as input data for micromecanical simulation models that allow the calculation of stress evolution in function of textures and along a complete loading cycle. The results show that the crystal and slip system reorientation hypothesis should be rejected on benefit of more traditional models of dislocation-point defects interaction.

Keywords: Low cycle fatigue, X-ray diffraction (XRD), texture, micro mechanical modeling, cyclic softening.

1 INTRODUCTION

It is known that well-annealed metals usually show cyclic hardening as a consequence of dislocation multiplication. Meanwhile the opposite is expected for initially hardened materials due to rearrangement of dislocation arrays and complex interactions with solutes and interstitials. However BCC metals, at low and medium deformation amplitudes, show an initial cyclic softening. This behavior is related with the strong interaction between dislocations and interstitial solute atoms [1-3]. HCP metals, such as Zirconium and its alloys Zircalloy-2 and Zircalloy-4, show a pronounced cyclic softening similar to the behavior observed for Titanium [4-6]. Recently, besides some other explanations of the kind “dislocation rearrangements” [7-8], some attention has been given in the literature to the so called “texture-rotation induced cyclic softening” model by which the imposed cyclic deformation would reorient the crystals to an orientation more favorable for prismatic slip [9-10]. The purpose of this Part II of the paper is to present some decisive texture measurement results and simulations rebating that model.

We study recrystallized Zircaloy-4 under low cycle fatigue tests. The starting material and samples tested at room temperature, medium (300 °C) and high temperatures (470 °C and 485 °C) were measured by
X-Ray and neutron diffraction. The results were analyzed by usual Orientation Distribution Functions and recalculated pole figures. Textures showed a gradual severity decrement with temperature and deformation but keeping the general pattern. The measured textures were used as input data for texture development simulation programs to calculate stress-strain curves. The simulations show that we cannot expect geometric softening arising from any of the measured textures when compared with the starting material. Texture development would definitively not be the reason for cyclic softening.

Crystallite reorientation during plastic deformation, or texture development, might contribute either to hardening or softening of a polycrystalline material in a so-called geometric phenomenon. Taylor factor variations can favorably or unfavorably contribute to ease further polycrystal deformation regardless of other hardening mechanisms like dislocation arrays, sub-grain boundaries, etc.

Geometric softening has been claimed to be one of the mechanisms able to create important sources of instabilities in plastic deformation processes [11-12]. However, there are very few examples, in monotonic plastic deformation tests, showing these phenomena translated macroscopically as an evident and effective decrement of the true stress-strain curve. Careful calculations and analysis are capable to demonstrate the separate contribution of intrinsic hardening of crystals belonging to a polycrystal and geometric softening stemming from preferential orientation development and significative Taylor factor diminishing. These phenomena are frequently apparent in heterogeneous deformation processes or transitory behaviors during thermo mechanical processes. Nevertheless, according to Choi et al., there would exist at least one case in which these phenomena would be evident, not in monotonic tests but in fatigue ones [9]. Based on fatigue studies performed in Zircaloy-4, they have proposed the so called “texture-rotation induced cyclic softening”. After this model, cyclic softening of the material would be produced by the rotation of textured crystals to an easier direction for prismatic slip. They calculated an average rotation of 15° of the (10\overline{1}0) direction around the <\overline{c}> axes that remains, standing by their description, perpendicular to the tensile axes. That reorientation would produce a 15% decrement of the peak tensile stress.

On the other hand, Armas et al., in Part I of this paper, have demonstrated that the cyclic softening observed in Zry-4 does not depend on the strain amplitude [8]. In this respect, if plastic deformation were the responsible for crystal reorientation leading to softening, a larger strain amplitude would convey more reorientation and consequently, larger and/or earlier softening. None is observed. Moreover, according to the same authors, the yield stress goes back to the initial values by simply annealing the already tested material. This fact would hardly mean texture going back to the initial grain orientation distribution but it rather suggests some kind of dislocation-solute interaction. Despite those truly strong experimental evidences are quite convincing by themselves, the purpose of the current paper is to inform a direct approach to the problem. Therefore, we measure the starting and after fatigue test textures and further calculate, by self-consistent polycrystalline codes, the expected stress-strain behaviors.

2 EXPERIMENTS

From Zircaloy-4 bars, following the ASTM B550 Grade 704 norms, shallow hourglass shaped specimens were cut with 8.8 mm gauge section and 21 mm length. Chemical composition is (in wt %): Sn-1.37, Fe-0.14, Cr-0.10, C-0.01, O-0.14, N-0.004, H-20 ppm, Zr-balance. The samples were tested in the recrystallized condition. Average grain diameter size was 20 microns. Total strain controlled cyclic tests with a strain range of 1.0 % and constant total strain rate of 2 x 10^{-3} s^{-1} were carried out using a fully reversed triangular wave. The tests were performed in air and always started in tension.

Typical cyclic behaviors are shown in Fig. 1: hardening at High Temperatures (HT) and softening at Room Temperature (RT). According to Choi et al. [2-8] one should assume that those behaviors would be the results of regular hardening at HT and geometric softening at RT. In such case the texture developments at HT and RT should be compatible with that assumption. Name of the samples and test temperatures of the measured samples are shown in Table I.
Most textures were measured in an X-ray Philips MPD diffraction machine with Eulerian cradle. We used Cu-Kα radiation monochromatized by a flat graphite crystal, Xe-CH4 gas proportional detector and a parallel plate collimator in the diffracted beam. Background and defocusing were also measured in a Zircaloy-4 random powder sample. Defocusing and background corrections and analysis were performed by popLA and Beartex softwares [13-14]. Pole figures allowed to calculate Orientation Distribution Functions, reconstruct pole figures and check coherency of experimental data. The cycled samples were cut in its central part and in the threaded head. Four 0.5 mm thick slices were cut from that central part of the sample allowing making a composite texture sample with enough scanning surface for X-ray measurements.

X-ray textures are representative of the orientations in the very middle of the gauge region which is supposed to be the most homogeneously deformed region. Texture results were obtained by measuring \{0002\}, \{10\overline{1}0\}, \{10\overline{1}T\}, \{10T\overline{3}\} and \{11\overline{2}0\} pole figures. Such profuse number of pole figures (PF) allowed the calculation of Orientation Distribution Functions (ODF) and recalculated PF’s with a high degree of accuracy and confidence by using different starting sets.

Some textures were measured by neutron diffraction. They are more representative of the bulk texture and they would be able to grasp some different details of texture modifications. A unique sample was cut from the central gauge part and another one from the threaded head. Both were placed in the sample holder of Tex-2 machine in GKSS Research Center - Geesthacht-Germany [15].

### 3 Texture Results

The X-ray textures are shown in Fig. 2. The texture of the “As Received” material was obtained from the holding threaded head of the Room Temperature sample. All exhibit the typical extrusion texture. The <c> axes are perpendicular to the sample longitudinal axis with the presence of a very weak orthotropic symmetry relic of the previous rolling deformation.

The textures measured by neutron diffraction show a similar behavior to that one shown by x-ray measurements. The diminishing severity of the textures is not limited to the very neighborhood of the fracture region but it goes all the way through the gauge length. Pole figures show a much better definition...
due to the superior penetration depth of neutrons and consequent higher averaging capabilities. Only the evolution of the maximum will be shown for AR and FRT samples for \{001\} and \{100\} pole figures.

Fig. 2 \{001\}, \{100\} and \{110\} recalculated Pole Figures for As Received, room temperature, medium temperature and high temperature fatigued samples.

Comparison between both measurement techniques allows to appreciate coincidences and homogeneity of the deformation behavior and textures. X-ray studies ensure that evolution of texture is not faster in the central zone than in the rest of the gauge length.

In all cases, qualitatively speaking, textures resemble the textures obtained by H. I. Choi et al. and D. H. Lee and S. I. Kwun \[9,10\]: that is the \(<c>\) axes almost exclusively perpendicular to the tensile axis. In such conditions activation of prismatic systems and consequent re-orientation of planes is undisputable. The evaluation of how much crystal re-orientation and how much the texture modification will influence the yield stress value in the tensile direction is a completely different and more difficult problem. The texture severity values obtained from the experimental and recalculated pole figures show a minor monotonic decrement for every pole together with the conservation of the general pattern of the texture; that is no sudden changes in component structure except for a minor change for FMT sample. Fig. 3 presents only recalculated intensities for main pole figures. At higher deformation temperatures the plastic deformation is larger for a given total deformation due mainly to the diminishing CRSS of every slip system. That larger accumulated plastic deformation softens even more texture intensities. Choi H.I et al. claim that re-orientation would be enough to diminish the yield stress due to the increment of the resolved stress applied on the prismatic slip planes \[9\]. The expected value, according to them, is around 15% for 15° of average rotation. In fact they do not provide more evidence than an incomplete sole \{10\} pole figure for before and after fatigue tests. The real re-orientation process is rather complex to be described by a single pole figure and simple average reorientation of prismatic planes. The phenomena are more of the kind of gradual smoothing probably due to intra-grain misorientations created by the cyclic deformation process. Besides, the results are far from such a large average re-orientation. \{10\} and \{1\} orientations, and particularly this last one, spread in a solid angle around the original orientation but without a net large reorientation. The same is true for the basal orientations.
4 MODELING THE POLYCRYSTAL YIELD STRESS

One way to evaluate the actual influence of every slip system and the effect of their plastic re-orientation on the yield stress of the polycrystal is by resorting to microcrystalline models. They allow obtaining the polycrystal average properties by accounting for the single crystal behavior and the texture. The current model has been described numerous times and its capabilities confirmed in many previous works. The interested reader is referred to them for details. It is a Self Consistent 1-site elastoplastic code that takes account of crystal and matrix anisotropy. Slip systems and twinning are considered as deformation mechanisms.

Measured textures allowed the design of representative collections of 1000 crystallites with the right volume fraction and orientation. Prismatic \{10\overline{1}0\} <1\overline{1}0\overline{1}> , Pyramidal \{10\overline{1}1\} <1\overline{1}23> slip systems and tensile and compression twinning \{10\overline{1}2\} <10\overline{1}\overline{1}> (TT1) and \{2\overline{1}\overline{1}\overline{2}\} <2\overline{1}\overline{1}\overline{2}> (CT1) were allowed, but because of the crystal orientation almost only prismatic slip systems were activated. Critical Resolved Shear Stresses were fixed at 100 MPa, 300 MPa and 210 MPa respectively. Elastic stiffness components for the single crystal were taken $C_{11} = 143.5$, $C_{12} = 72.5$, $C_{13} = 65.4$, $C_{44} = 32.1$ and $C_{66} = 35.5$, all values given in GPa. Fig. 4 shows the almost exact superposition of all simulated stress-strain curves independently of the starting texture. Fig. 5 shows a whole cycle and a quarter tensile stroke showing the hardening effect starting from the AR texture data.

Fig. 4 Simulation of the Stress-Strain curves along one tensile stroke for the different starting textures.
5 DISCUSSION AND CONCLUSIONS

Coincidence between all curves in Fig. 4 is rather artificial because we assume that the ratio between all different CRSS and absolute values are constant for all temperatures. If we try to catch the influence of texture, comparisons should be made for the same single crystal properties and that cannot be done because each cyclic test is performed at different temperature. In that sense the stress axes of Fig. 4 can be considered normalized with respect to the room temperature CRSS. In any case, whichever the temperature influence over the material hardening (softening), the model is about calculating texture dependence of yield stresses and not temperature dependences.

For low plastic deformations (v.g. less than 1-2 %) one can neglect the hardening due to dislocation arrangements and the sole visible effect should be due just to crystal re-orientation geometric softening (hardening) if it happens to exist. For cyclic deformation processes, where low cyclic strains can accumulate very large total deformations and consequently create very complex dislocation structures, large hardening effects may arise. But we do not even have to approximate the actual value of the yield stress because texture induced softening (hardening) should be anyhow visible in the simulations performed for different starting textures. Just by staying close to reasonable values we may trust the assumed single crystal hardening law to evaluate the variation in yield stress expected from the texture variations. Far from being a limitation, even a simulation performed under the assumption of small plastic strains should render behaviors representative of...
the re-orientation model from Choi H.I. et al. [9]. We have used a linear hardening resembling the typical behavior at low plastic deformations.

Dislocation hardening or back stress and temperature differences between CRSS, is not what is under discussion between both models. Discussion is about the nature of the observed changes in friction stress which are usually connected with temperature or time dependent effects. Choi H.I. et al. [9] claim that the original lattice strain, main part of the friction stress, is by itself responsible of the softening by the simple provision of changing the texture. Meanwhile according to Armas et al. (Part I) [8] the unlocking of dislocations from their oxygen interstitial solute atoms during cycling is responsible for such behavior. This mechanism is contributing also to the friction stress but it would not be orientation dependent. None of them is arguing about long range stresses, back stresses or regular dislocation hardening phenomena. So, the fact that we do not deal with very fine details of hardening micro mechanisms in our simulation is not precluding the prediction success of the model. Whichever the hardening law, even one of the kind “dislocation-point defect interaction”, the current changes in texture are very small and we do not expect large texture dependences. All simulations, either for HT or RT textures, show the usual hardening behavior expected from back stresses building up due to dislocation arrays.

Normal cyclic hardening exhibited by Fig. 5 also shows that regular dislocation hardening cannot be compensated, less even reversed by geometrical softening or development of internal stresses due to prior deformation.

Experimental and simulation results are not consistent with the hypothesis of the “texture-rotation induced cyclic softening” model, that is geometric softening. Friction stress decrement due to dislocation unlocking from oxygen interstitials during cycling appears to be the most trustable model, as claimed by Armas et al. (Part I) [8].

6 ACKNOWLEDGEMENTS

This work was supported by the Agencia Nacional para la Promoción de la Ciencia y Técnica (ANPCYT), the Consejo Nacional de Investigaciones Científicas y Técnicas from Argentina and Fundación Antorchas. The authors acknowledges helpful discussions about simulation strategies with Dr. Pablo A. Turner.

7 REFERENCES


