Micromechanical approach of visco-plastic behaviour of recrystallized Zircaloy-4 at 400°C

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Aims of the study

► Experimental investigations of anisotropic visco-plastic behavior of recrystallized Zircaloy-4 at 400°C
  ◆ … On macroscopic scale (mechanical tests)
  ◆ … And also on microscopic scale (TEM observations)

► Development of multiscale modelling based on observed deformation mechanisms [1,2]

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A polycrystalline modeling of the mechanical behavior of neutron irradiated zirconium alloys
Fabien Onimus and Jean-Luc Béchade

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Toward a better understanding of mechanisms responsible for size evolution of fuel rods
Material of the study

- Crystallographic texture

Poles figures (EBSD analysis)

- Grain size: Mean diameter around 5 μm

Crystallographic texture is mainly responsible for viscoplastic anisotropy of Zirconium products
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Priser et al – Session 2 : Fabrication and mechanical properties
Experimental set up: Creep tests

- Creep Advanced Testing [1]
  - Axial load up to 5 kN
  - Internal pressure up to 200 bar
  - Radiative furnace with controlled environment
  - Laser extensometers
    - Axial and hoop strain

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[1] Experimental creep behaviour determination of cladding tube materials under multi-axial loadings
Catherine Grosjean, Dominique Poquillon, Jean-Claude Salabura and Jean-Marc Cloué
Experimental set up : Relaxation tests

- **Gleeble® device**

- Axial load up to 50 kN
- Joule heating
- Secondary vacuum
- LVDT extensometer
  - Hoop strain only
Experimental results

$[T=400^\circ C]$
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TEM method

Fragments of tested Zy4-RX guide tubes
Mechanical grinding
Electrolytic polishing

Cristallographic analysis of each grain
(ex: (0002) pole figures)

A statistical and experimental approach of the physical mechanisms contributing to grain deformations.

TEM investigations on 50 grains for each specimen
Glide of dislocations (mostly with a screw character) lies in the prismatic planes.

Very few secondary slip systems, and no evidence of climb mechanisms were observed.

One, two or three prismatic slip systems can be simultaneously activated within a grain.

Considering grains with prismatic slip, cross-slip has 40% chances to be activated.
Creep and relaxation: main differences

Several grains with very narrow dislocation dipoles were observed in the crept specimen only.

Distribution of dislocation densities

More dislocation substructures were observed in the crept specimen (18%) than in the relaxed specimen (5%).

Although both specimens exhibit the same macroscopic plastic strain level, deformation distribution is less homogeneous inside the crept sample than in the relaxed sample.
**Activation volume analysis**

- Activation volume is the sensitivity of plastic strain rate to stress (viscosity)
- Apparent volume is defined as the macroscopic sensitivity

\[ V_{app} = k_B T \left( \frac{\partial \ln |\dot{\varepsilon}_{\theta\theta}|}{\partial \Sigma_{zz}} \right) \]

**Differences in activation volumes come from sensitivity of inter-granular plastic accommodation to strain rate**
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Outline

- Mechanical testing
- TEM observations
- Multiscale modelling
Micromechanical approach

**Modelling strategy**

From plasticity mechanisms to polycrystal behavior

1. Localization step
2. Single crystal plasticity law
3. Representation step

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Single crystal behavior

- Annihilation
  - [Cross-slip]
  
  \[ P_{CS} = \beta_0 \exp \left( \frac{\max_{s \in P} \left| \tau_{\pi_1, <a>} \right| - \tau_{\pi_1, <a>}^\mu}{k_B T} \right) V_{CS} \]

  \[
  \text{if } s \in P : \quad \dot{\rho}_s = \frac{|\dot{\gamma}_s|}{b} \left\{ \frac{1}{\lambda} - 2y_s P_{CS} \rho_s \right\}
\]

  \[
  \text{if } s \in \pi_1 : \quad \dot{\rho}_s = \frac{|\dot{\gamma}_s|}{b} \left\{ \frac{1}{\lambda} + K_{CS} P_{CS} \rho_P - 2y_s \rho_s \right\}
\]

- Production
  - [Frank & Read mechanism]

- Work-hardening
  - [Orowan law]

\[ \tau_{\mu}^{(s)} = \tau_0 + \alpha \mu b \sqrt{\sum_{r \in S} \rho_r} \]
Cross-slip mechanism

- Description of Cross-slip mechanism
  
  - One prismatic dislocation can cross-slip on only 2 out of 3 pyramidal planes ($P \rightarrow \pi_1$)
  - Increases critical annihilation length production
    - Softening mechanism
  - Increases dislocations production on pyramidal systems
    - Hardening mechanism
Polycrystal behavior

Transition scale rule

- “Self-consistent” approach of the polycrystal behavior

For each crystallographic phase $g$ ($\beta$ rule [Pilvin, 1990]):

$$
\sigma_g = \sum + 2\mu(1 - \beta)(B - \beta)_{g}
$$

with:

$$
\beta = \frac{\epsilon_{p}}{\epsilon_{g}} - D(\beta_{g} - \delta\epsilon_{p})\parallel\epsilon_{g}
$$

\[\Sigma = \sum_{g\in G} f_{g}^{vol} \dot{\varepsilon}_{g}^{vp} \]

\[\dot{E}_{vp} = \sum_{g\in G} f_{g}^{vol} \dot{\varepsilon}_{g}^{vp} \]
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Model / Experiment comparison

Creep curves

\[ \varepsilon_{zz} \text{ and } \varepsilon_{\theta\theta} \text{ vs time for different biaxiality of the loading} \]

- \( \beta = +\infty \)
- \( \beta = 1 \)
- \( \beta = 0 \)

Relaxation curves

Axial stress vs hoop strain
Cross-slip probability and dislocations density are strongly dependent on loading directions.
Conclusions

- Experimental investigations of anisotropic mechanical behavior of recrystallized Zircaloy-4 at 400°C
  - On macroscopic scale using mechanical tests (creep and relaxation)
  - On microscopic scale with TEM analysis

- Numerical investigations with a micromechanical approach build on TEM observations
  - Prismatic and pyramidal slip + cross-slip

- Good way for modelling the mechanical behavior
  - But further developments of the model are necessary ...
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THANK YOU FOR YOUR ATTENTION

Chengdu (成都), Monday May 10\textsuperscript{th}, 2010
16\textsuperscript{th} International Symposium on Zirconium in the Nuclear Industry
Session 2 : Fabrication and mechanical properties
Cross-slip and anisotropic creep behavior

Strain-rate equi-potential creep surface and cross-slip mean probability

\[
d\dot{\varepsilon}_{eq}^{II} = \frac{2}{3} \left( \dot{\varepsilon}_{\theta\theta}^{II^2} + \dot{\varepsilon}_{zz}^{II^2} \right)
\]

\[
\langle P_{CS} \rangle = \sum_{\varphi \in G} f_{v}^{\varphi} \langle P_{CS}^{\varphi} \rangle
\]

- Dichotomic search of equi-potential creep surface
- Anisotropic contribution of cross-slip to stage II

Very tough modelling around equi-biaxial direction

Anisotropic mean probability of cross-slip

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\[
\frac{d\varepsilon_{eq}^{II}}{dt} = \sqrt[3]{\frac{2}{3} \left( \dot{\varepsilon}_{\theta\theta}^{II^2} + \dot{\varepsilon}_{zz}^{II^2} \right)}
\]

\[
\langle P_{CS} \rangle = \sum_{\varphi \in G} f_{v}^{\varphi} \langle P_{CS}^{\varphi} \rangle
\]