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Micromechanical modelling of creep of zirconium alloys

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ABSTRACT

Modelling irradiation effects on the mechanical behaviour of polycrystalline zirconium alloys in Pressurized Water Reactors needs to develop a micromechanical approach in the elastic-viscoplastic range. We adopt an incremental formulation using at each step the Laplace-Transform technique. This new formulation takes into account evolutions of intragranular internal variables. First simulations prove that this new approach yields better predictions than former ones.

1. INTRODUCTION

Zirconium alloys are used for guide tubes and grids of Pressurized Water Reactors' fuel assemblies. Insuring the geometrical stability of these components needs to model the behaviour of zirconium alloys submitted to thermomechanical loading and irradiation. Moreover, given that irradiation effects result from low scale mechanisms, micromechanichal approaches are essential to perform reliable predictions.
First, a relevant description of irradiation effects at the crystal level is needed. Former work [1] based on a physical description of interaction between neutrons damage and dislocations has led to a general formulation of the constitutive equations of single crystals which prove to be of an elastic-viscoplastic nature and need internal parameters.
The second stage concerns the scale transition from the single crystal to the polycrystal. Adequate schemes were proposed in the elastoplastic range [2] while until recently simplified methods only were available in the elastic-viscoplastic range.
This paper focuses on this second step. We present a new formulation of the self-consistent scheme in the elastic-viscoplastic domain including the evolution of intragranular internal variables. We then compare results obtained from this approach with former ones and we report preliminary simulations concerning zirconium alloys.

2. THE MICROMECHANICAL APPROACH

Let us consider a polycrystalline volume element. This volume sample is submitted to macroscopically homogeneous stress Σ and strain E under neutron irradiation (fluence Φ and flux ϕ). We aim at deriving the overall behaviour of this sample from the single crystal behaviour (in the framework of small strains analysis).

2.1 Single crystal behaviour

According to former studies [1], the strain rate of an irradiated crystal under stress σ includes three different parts,

$$\dot{\varepsilon} = \dot{\varepsilon}_e + \dot{\varepsilon}_c + \dot{\varepsilon}_{irr} \qquad (1)$$

$\dot{\varepsilon}_e$ is the elastic part of the strain rate, namely,

$\dot{\varepsilon}_e = s\dot{\sigma}$ with the elastic compliances s.

$\dot{\varepsilon}_c$ is the viscoplastic strain rate associated with thermal creep.

Assuming that the thermal creep is controlled by dislocation glide, $\dot{\varepsilon}_c$ reads,

$\dot{\varepsilon}_c = \sum_s \dot{\gamma}_s^0 \, sh\left(\frac{R_s \sigma}{\tau_s^0}\right) R_s$, where R_s denotes the orientation tensor of the system (s), $\dot{\gamma}_s^0$ its reference shear strain and τ_s^0 its reference shear stress. The reference shear stress τ_s^0 depends on hardening effects but it also depends on the fluence Φ .

$\dot{\varepsilon}_{irr}$ is the strain rate due to irradiation.

Applying Woo's kinetic theory [3], this term reads,

$\dot{\varepsilon}_{irr} = \sum_s \rho_s (V_1^s + V_2^s \sigma)(k_1^s \frac{\underline{b}^s}{\|\underline{b}\|} + k_2^s \underline{n}^s) \times \underline{b}^s$, where (s) is a moving dislocation family, $\underline{b}^s$ its burgers vector and $\underline{n}^s$ the normal to its glide plane. v_1^s and v_2^s are constants which depend on the fluence Φ , the flux ϕ , the temperature T and the dislocation family (s). k_1^s and k_2^s are geometrical terms.

Finally, a general expression of the elastic-viscoplastic strain rate is the following :

$$\dot{\varepsilon} = s\dot{\sigma} + g(\sigma, \underline{\alpha}) \qquad (2)$$

with $\underline{\alpha}$ a set of N internal variables given by : $\dot{\underline{\alpha}} = \underline{h}(\sigma, \underline{\alpha}, T, \Phi, \dot{\Phi})$ (3)

For instance, $\underline{\alpha}$ would be the dislocations density, the reference shear stresses, the shear rate on each slip system... To reduce computing times, the number of internal variables needs to be decreased. Therefore, the relevant internal variables alone would have to be introduced. Without specifying these variables, we now present a general homogenization procedure which takes this set of internal variables into account when g and $\underline{h}$ are non linear functions (T, Φ and $\dot{\Phi}$ can be considered as fixed).

2.2 A self-consistent homogenization scheme

This scheme which is known to be relevant for polycrystals is based on an extension of Hill's treatment of the rate independent regime to the rate dependent's one [2].
The stress and strain fields (σ,ε) are supposed to be uniform in each single crystal with,

$$<\sigma>=\Sigma \quad \text{and} \quad <\varepsilon>=E$$

(where $<\ >$ denotes the average over all the phases.)

Linearization procedure :
Given a time t_n, we suppose that the local and overall responses have been determined for any time t prior to t_n. The linearization of equations (2) and (3) in each phases leads to,

$$\dot{\varepsilon}(t) = s:\dot{\sigma}(t) + m_n\sigma(t) + n_n\underline{\alpha}(t) + \dot{\varepsilon}^0_n(t) \tag{4}$$

$$\dot{\underline{\alpha}}(t) = p_n\sigma(t) + q_n\underline{\alpha}(t) + \dot{\underline{\alpha}}^0_n(t) \tag{5}$$

with,

$$\left|\begin{array}{ll} m_n = \dfrac{dg}{d\sigma}[\sigma(t_n),\underline{\alpha}(t_n)] & n_n = \dfrac{dg}{d\underline{\alpha}}[\sigma(t_n),\underline{\alpha}(t_n)] \\ p_n = \dfrac{dh}{d\sigma}[\sigma(t_n),\underline{\alpha}(t_n)] & q_n = \dfrac{dh}{d\underline{\alpha}}[\sigma(t_n),\underline{\alpha}(t_n)] \end{array}\right.$$

In order to satisfy the constitutive laws for $t<t_n$, $\dot{\varepsilon}^0_n$ and $\dot{\underline{\alpha}}^0_n$ must be taken in the form :

$$\begin{aligned}\dot{\varepsilon}^0_n(t) &= g(t_n) - m_n\sigma(t_n) - n_n\underline{\alpha}(t_n) \\ &\quad + [g(t) - g(t_n) - m_n(\sigma(t) - \sigma(t_n)) - n_n(\alpha(t) - \alpha(t_n))][1 - H(t - t_n)]\end{aligned} \tag{6}$$

$$\begin{aligned}\dot{\underline{\alpha}}^0_n(t) &= \underline{h}(t_n) - p_n\sigma(t_n) - q_n\underline{\alpha}(t_n) \\ &\quad + [\underline{h}(t) - \underline{h}(t_n) - p_n(\sigma(t) - \sigma(t_n)) - q_n(\underline{\alpha}(t) - \underline{\alpha}(t_n))][1 - H(t - t_n)]\end{aligned} \tag{7}$$

where H(t) is the unit step function.

Homogenization procedure :
It has been shown [4] that equations (4) and (5) yield,

$$\varepsilon(t) = [s_n \otimes \dot{\sigma}](t) + \varepsilon^0_n(t) \tag{8}$$

($\otimes$ denotes the Stieljes convolution product such that, $[s_n \otimes \sigma](t) = \int_0^t s_n(t-u)\dot{\sigma}(u)du + s_n(t)\sigma(0)$)

were s_n will be evaluated later. $\varepsilon^0_n(t)$ does not depend on the loading conditions beyond t_n so that it is a true eigenstrain.

Consequently, each phase has a maxwellian linearized behaviour with eigenstrain and the overall behaviour obeys [5],

$$E(t) = [S_n \otimes \Sigma](t) + E^0_n(t) \tag{9}$$

with,

$$E^0_n(t) = <[{}^tB_n \otimes \varepsilon^0_n](t)> \tag{10}$$

$$\varepsilon(t) - E(t) = -[M_n \otimes (\sigma - \Sigma)](t) \tag{11}$$

(where ${}^tB_n$ is the transposed tensor of the stress concentration tensor B_n when no eigenstrains are present and M_n is Hill's constraint tensor)

Once the stresses are deduced from (11) from time t_n to time $t_{n+1}=t_n+\delta t$, we derive the evolution of internal variables through (3). Consequently, we obtain an incremental procedure which allows us to derive at each step the local and overall responses during the time interval $[t_n;t_{n+1}]$.

Numerical method :

To perform the calculations, we use the Laplace-Carson Transform technique : $s_n^*(p) = p\int_0^{+\infty} s_n(t)\exp(-pt)dt$ is the symbolical viscoelastic local compliance and reads,

$$s_n^*(p) = s + \frac{1}{p}m_n + \frac{1}{p}n_n(pI - q_n)^{-1}p_n \qquad (12)$$

(I denotes the second order unit tensor in a N*N space)

and the overall symbolical compliance is given by,

$$S_n^*(p) = < s_n^*(p)\, B_n^*(p) > \qquad (13)$$

The symbolical stress concentration tensor $B_n^*(p)$ of the crystal (r) is given by,

$$B_n^*(p) = [M_n^*(p) + s_n^*(p)]^{-1}[M_n^*(p) + S_n^*(p)] \qquad (14)$$

Defining $S_{esh}^*(p)$ the symbolical Eshelby tensor [6] associated to the elastic one by the correspondence principle which depends on $S_n^*(p)$ and the shape of the crystal (r), Hill's constraint tensor reads,

$$M_n^*(p) = [I_4 - S_{esh}^*(p)]^{-1}S_{esh}^*(p)\, S_n^*(p) \qquad (15)$$

(I_4 denotes the identity tensor)

The last difficulty consists in inverting the symbolical functions given that the fully analytic inversion is untractable. That is why we use an approximate inversion procedure, namely the collocation method [7]. Each symbolical function is approximated by a finite Dirichlet series of the form,

$$S_n(t) = \sum_k b_n^k \exp(-\frac{t}{\tau_n^k}) \qquad (16)$$

3. PRELIMINARY APPLICATIONS

We consider an unirradiated polycrystal and we neglect hardening effects in each crystal. Each phase is represented by a spherical inhomogeneity.

As in part 2, we suppose that inelastic strains are due to dislocation glide only so that the single crystal constitutive equations read,

$$\dot{\varepsilon} = s:\dot{\sigma} + \sum_s \dot{\gamma}_s(\sigma)R_s \qquad (17)$$

with the shear strain rate $\dot{\gamma}_s(\sigma)$ on system (s) given by,

$$\dot{\gamma}_s(\sigma) = \dot{\gamma}_s^0\,[\frac{R_s\sigma}{\tau_s^0}]^n \qquad (18)$$

3.1 Comparisons with former approaches

Taylor's approach [8] lies on the assumption of uniform strain in the whole volume sample, namely,

$$\varepsilon = E \text{ in each phase.}$$

Because of this assumption, grain to grain interactions are overestimated so that Taylor's predictions turn out to be too stiff.

In order to take viscoplastic strain heterogeneities into account, Weng [9] argued that Kröner's elastoplastic self-consistent scheme, which was known to be unadequate in that case, was actually rigorously valid in the rate-dependent range. It has been shown [10] that this statement, which leads to take elastic intergranular interactions into account, is based on the incorrect assimilation of viscoplastic strains to eigenstrains, so that internal stresses are strongly overestimated and the strain heterogeneity underestimated. As a matter of fact, predictions derived from this model are very close to Taylor's ones. [11].

On Fig. 1, we compare predictions of a uniaxial tension creep test derived from our model with Weng's one. The material considered here is an untextured face centred cubic (FCC) polycrystal with isotropic elasticity and viscoplastic glide occurring on octahedral slip systems.

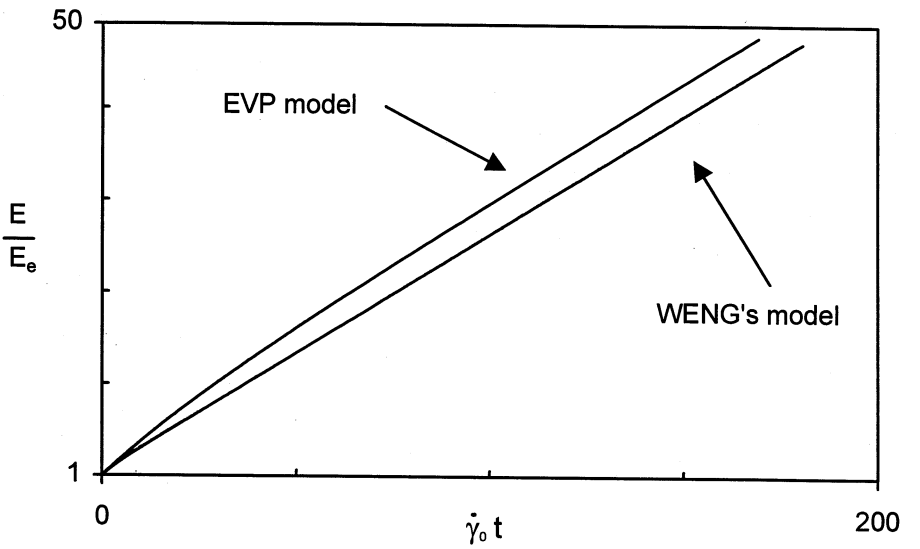

Fig. 1: Comparison between the tensile creep response of an FCC polycrystal, as predicted from Weng's treatment and ours ("EVP model")

(E_e is the elastic overall strain, $\dot{\gamma}_0$ a reference shear strain rate and t the time)

It is satisfying to notice that our prediction is softer than Weng's one, as expected. Therefore, such as Hill's approach compared to Kröner's one in the elastoplastic range, our method improves the description of the elastic-viscoplastic grain to grain interactions with respect to former ones.

3.2 Steady creep of untextured zirconium alloys

We next consider an untextured zirconium alloy polycrystal submitted to the constant macroscopic stress Σ. As in former studies [12], we assume that thermal creep is controlled by dislocation glide on prismatic, basal and pyramidal slip systems.
We assume that all slip systems have the same stress exponent n and the same reference shear rate $\dot{\gamma}_0$. Moreover, we adopt the following values for the reference shear stresses [12].

Slip systems	Prismatic slip	Pyramidal slip	Basal slip
Reference shear stresses (Mpa)	$\tau_{pr}^0 = 40.0$	$\tau_{py}^0 = 60.0$	$\tau_b^0 = 120.0$

table 1 : Reference shear stresses adopted.

In the steady regime, the macroscopic strain rate reaches a constant value. In the case of radial loading, this steady strain rate is given by [13],

$$\dot{E}eq = \dot{\gamma}^0 \left(\frac{\Sigma eq}{\Sigma 0}\right)^n \qquad (19)$$

where the effective reference stress Σ_0 depends only on n, the values of the reference shear stresses and the loading path.
On Fig. 2 we compare the variations of the effective reference stress with the non-linearity factor n as predicted from our approach with Weng's ones*. In this case, Weng's predictions and Taylor's ones are identical.

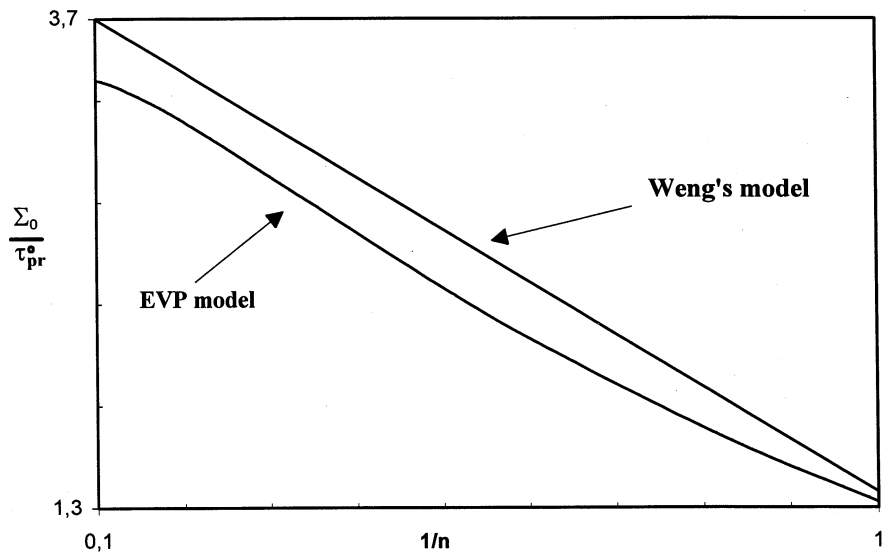

Fig. 2 : Effective creep reference stress as predicted by Weng's treatment and ours ("EVP" model)

* An isotropic distribution of crystalline orientations was kindly given by B. BACROIX (LPMTM, CNRS UPR9001, Univ. PARIS13 (FRANCE)) to perform these simulations.

Now again, our results are softer than Weng's one. So, our method leads to improved micromechanical predictions for hexagonal closed packed (hcp) polycrystals too.

CONCLUSION

We have proposed a micromechanical approach well suited to elastic-viscoplastic constitutive behaviours. First results show that this scheme yields better predictions than former ones.
Applications of this approach to effects of texture and intragranular hardening in zirconium alloys would require further developments within the framework proposed here.
On the other hand, we have proposed a general scheme with internal variables to take irradiation effects into account. Reduction of computing times and specifications of relevant internal variables to describe irradiation damage will give access to a comprehensive modelling of the thermomecanical behaviour of zirconium alloys in Pressurized Water Reactors.

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