MODELING THE MECHANICAL BEHAVIOUR OF CANDU© FUEL CLADDING

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Abstract

Models for the mechanical behaviour of fuel cladding were developed in the period 1973-1983 by staff at AECL CRNL. The models for the mechanical properties of fuel cladding during normal operation were a by-product of programs during the period 1970-1975 to understand the origin of fuel-cladding defects caused by power ramps at Douglas Point and Pickering A. Models for accident coonditions were, initially, based heavily on mechanical properties data generated by McGill University and Westinghouse Canada under contract to AECL in the late 1960's and early 1970's and attempts to interpret the data in terms of the underlying deformation mechanisms. The model for normal operating conditions was embodied in the ELESTRES/ELESIM series of codes, and the models for accident conditions were embodied in NIRVANA.

1. INTRODUCTION

The development of numerical models for the behaviour of CANDU© fuel cladding during normal operation and during hypothetical accident conditions became a priority for AECL in the early to mid-1970s, with a major effort on physical and chemical properties of the UO_2 under radiation. Models for the mechanical behaviour of the fuel cladding were initially an adjunct to this effort, but several of the metallurgists at CRNL who worked on zirconium alloys for fuel cladding and pressure tubes had independently been modeling the mechanical behaviour of these alloys to understand power ramp fuel defects and the development of improved pressure tube materials. Their subsequent involvement in the fuel modeling effort grew out of coffee table conversations with fuel experts in Building 375 at CRNL, especially Ross MacEwan and Mike Notley, who along with Archie Robertson encouraged their participation in the fuel modeling effort.

2. NORMAL OPERATING MODEL

The development of realistic models for the mechanical behaviour of fuel cladding during normal operation grew out of the program put in place in 1970 to understand the early fuel failures, initially in Douglas Point, and subsequently Pickering A. The work is summarized in Reference [1]. The defects were caused by an increase in power after a period of burn-up at a lower power. One proposed explanation for the defects was plastic instability (necking) of the cladding associated with localized stress and loss of necking resistance due to irradiation damage in the cladding, see Reference [2], e.g.(the latter would account for the requirement of a period of burn-up prior to the power increase). The general numerical study of plastic instability was initiated by Coleman [3], and subsequently he collaborated with Holt and Hosbons to model the development of plastic instability in tensile tests [4] and the rather severe the effects of irradiation damage on the resistance to necking [5], using the expression:

$$\sigma = W(\Phi, \varepsilon)\dot{\varepsilon}^m \varepsilon^n$$

where σ is the applied stress, ε is the plastic strain, $\dot{\varepsilon}$ is the plastic strain rate, Φ is the fast neutron fluence, $W(\Phi, \varepsilon)$ represents the removal of radiation damage by dislocation sweeping [2], m is the strain rate sensitivity, and n is the work hardening exponent.

The key parameters controlling plastic instability were W, m and n. Necking initiates depending upon W and n, high positive values delaying necking. High values of n and m two inhibit necking according to [6]:

$$\frac{\Delta\dot{\varepsilon}}{\dot{\varepsilon}} = -\frac{1}{m} \cdot \frac{\Delta A}{A}\left(1 - \frac{n}{\varepsilon}\right)$$

where $\frac{\Delta\dot{\varepsilon}}{\dot{\varepsilon}}$ is the rate of necking at a discontinuity with an area differing by ΔA from the area of the bulk of the specimen, A.

The value of W proved decrease with strain at low strains, n was low and m also very small (i.e., <0.05) in irradiated Zircaloy-4 at reactor operating temperatures [2]. This showed that fuel cladding would be susceptible to failure at very low plastic strains (<1%), especially if the strain was localized over cracks in the fuel. Although it was subsequently shown that fission products were also necessary to cause power-ramp defects [1], this did forewarn of the possibility of sheath splitting in the event of a large, rapid, power insertion.

To represent fuel cladding deformation, the model was normalized to an extensive dataset for the properties of Zircaloy-2 cladding [7] and extended to cover primary creep [8] and irradiation creep at low stresses [9] where the total plastic strain rate was the sum of the three components, i.e.,

$$\dot{\varepsilon}_t = \dot{\varepsilon}_{pl} + \dot{\varepsilon}_{pr} + \dot{\varepsilon}_{ir}$$

where the subscripts *t, pl, pr, ir* denote total, plasticity, primary creep and irradiation creep respectively. The equation describing each is an expension of that for plasticity alone, i.e.,

$$\sigma = W_s(\Phi, \varepsilon_s)\phi_s^q \dot{\varepsilon}_s^m \varepsilon_s^n$$

where ϕ is the fast neutron flux and s represents *pl, pr,* or *ir*, and for each subscript *W, q, m* and *n* are different. This model proved reasonably successful at predicting sheath strain and fission gas release in CANDU fuel [10] and was adopted to represent the mechanical behaviour of the fuel cladding in the ELESIM/ELESTRESS series of fuel modeling codes, where it is still in use.

3. ACCIDENT MODEL

By the mid 1970's nuclear plant designers, plant owners and regulators were becoming increasingly concerned with the potentially large consequences of relatively improbable accidents such as loss of coolant and loss of emergency coolant combined with loss of containment. Although it was recognized that the fuel cladding would deform as the coolant pressure dropped, and fuel and cladding temperatures increased, it was expected initially that the cladding would remain intact and contain the fission products. This was expected to be confirmed by modeling the mechanical behaviour of the cladding under such conditions.

This is a much more complicated problem that the modeling of deformation at normal operating temperatures because, as the cladding heats up, it undergoes annealing of residual cold work and radiation damage, recrystallization, grain growth and transformation from α (hcp) to α + β (bcc) to β and several deformation processes must be considered.

3-1. Dislocation Creep.

Holt and Sills [11] collaborated to develop a model for deformation of the α-phase, based on high temperature deformation data for Zr-Sn alloys developed at McGill University under contract to AECL [12,13] and Holt [14] developed a model for deformation of the β-phase based on creep data developed by Clendening at Westinghouse Canada [15], again under contract to AECL, and Clay and Redding at CEGB Berkeley Laboratories [16]. Both models were similar and contained a parameter, σ_I, that represented the history of the material prior to the start of deformation. The strain rate was expresses as:

$$\dot{\varepsilon} = C_j \exp\left(-Q_{j1}/TR)\right)\sigma_*^k$$

$$\sigma_* = \sigma - \sigma_i$$

$$\dot{\sigma}_i = \partial\sigma_i/\partial t = U_j E_j \dot{\varepsilon}/\sigma_i^p - B_j/T\sigma_i^q\sigma_*^h \exp\left(-Q_{j2}/RT\right)$$

$$\sigma_i = \int \dot{\sigma}_i dt$$

In these expressions Q_1 and Q_2 are activation energies for creep and recovery, σ_* and σ_i are the "effective" and internal stresses, C, U, B, k, p, q, h and R are constants (R is the gas constant), $\dot{\sigma}_i$ is the rate of change of σ_i with respect to time, E is the elastic modulus, t is time and T is absolute temperature. All the parameters had different values for the α-phase and the β-phase as denoted by the subscript, $j = \alpha$ or β.

This expression allowed the calculation of deformation under transient (stress and temperature) conditions for each phase and also allowed the continuous evaluation of n and m the work hardening exponent and strain rate sensitivities, which, as mentioned above, largely control whether necking occurs.

Sills and Holt [17] subsequently combined these models with a number of others, representing the metallurgical phenomena that occur during heating of Zircaloy-4, under stress to temperatures up to 1700K. These include:

3-2. Athermal Glide.

When very high stresses are applied (above a certain critical stress, $\sigma_* \cong 2x10^{-3}E$), the strain rate no longer obeys the temperature sensitive power law given above, but is instantaneous and limited by work-hardening [18], i.e.,

$$\dot{\sigma}_a = \dot{\sigma}_i = U_j E_j \dot{\varepsilon}$$
$$\sigma_a = 2x10^{-3} E_j + \int \dot{\sigma}_i dt$$

where U_j is the work hardening coefficient.

Dislocation creep is assumed to occur simultaneously with athermal glide and the strain rates are additive. In this regime the strain rate sensitivity is negligible, and if radiation damage has not yet recovered the ductility will be low.

3-3. Grain/Phase Boundary Sliding.

This model is included because deformation mechanisms with a low sensitivity to stress (typical of sliding mechanisms [19,20]) are observed in the high α and in the α+β phase fields, for example at low stresses during steady state creep of Zircaloy-4 fuel cladding at 1123 and 1173K [15]. The rate is given by:

$$\dot{\varepsilon}_{slide} = C_1 \left(\frac{\sigma_a}{E}\right)\left(\frac{b}{d}\right)^2 \exp(-Q_3 / RT)$$

where C_1 is a constant, b is the lattice spacing, d is the grain size and Q_3 is the activation energy for self diffusion (bulk or boundary).

3-4. Phase Transformation Strain.

On transformation from α to β on heating and from β to α on cooling the phase transformation obeys the Burgers relationship, which results in a significant microscopic shear [21]. As suggested by

Greenwood and Johnson [22], when the phase transformation occurs under stress, the direction of this shear is biased by the stress, resulting in a macroscopic deviatoric strain. This is represented by:

$$\dot{\varepsilon}_{trans} = C_2 \sigma_a \dot{f}_\alpha$$

where C_2 is a constant and $\dot{f}_\alpha$ is the rate of change of the volume fraction of α.

The occurrence of this phenomenon was verified by examining Clendening's experimental records for specimens tested isothermally in the two phase regime and cooled under load [15]. Examination of for isothermal tests in the two showed that acceleration in the strain rate was observed as the specimens cooled through the phase transformation [23].

In addition to the four deformation mechanisms cited in sections 3-1 to 3-4, it is necessary to model the changes in the microstructure (radiation hardening, hardening from cold work, recrystallization, grain size and the phase transformation.

3-5. Recovery/Recrystallization.

At the initiation of an accident transient, fuel cladding contains residual cold-work and radiation damage. In the dislocation creep and athermal glide models this in represented by an initial value of σ_i corresponding to the difference in yield stress between the irradiated cladding and unirradiated, fully recrystallized cladding (corrected for temperature in proportion to the elastic modulus). Recovery and recrystallization are modeled dynamically based on data by Lee[23]. The rate of recrystallization is given by:

$$\dot{f}_u = f_u C_3 \exp\left(-Q_r / RT\right)$$

Where f_u is the unrecrystallized fraction, $\dot{f}_u$ is the rate of change of the unrecrystallized fraction, C_3 is a constant and Q_r is the activation energy for recrystallization. This model gave a good fit over a wide range of data recrsyatllzation data from isochronal annealing for times up to 64 hours [24] (recrystallization temperature of 1025 K) to dynamic heating at rates up to 25 $K.s^{-1}$ [25] (recrystallization temperature of 1225 K).

3-6. Grain Growth

No dynamic grain growth model was developed as such. In the model, the grain size was increased from 3 to 10 μm as recrystallization proceeded (itself a dynamic process as described in section 3-5) and from 10 to 100 μm as the phase transformation from α to β occurred (see section 3-7).

Because the β to α transformation results in a Widmanstätten structure [26] that is not susceptible to grain or phase boundary sliding, the grain size was assumed to remain at 100 μm during cooling.

3–7. α to β Phase Transformation

Initially [16], the equilibrium phase distribution was assumed to apply, based upon the equilibrium data of Holt [26,27], but subsequently a dynamic model was developed by Holt, Sills and Sagat [28] based on the kinetic data of Holt and of Chung, Gardé and Kassner [29]. The rate of transformation is given by:

$$\dot{f}_\alpha = sC_4\left(T_e - T\right)\exp\left(-Q_t / RT\right)$$

where s is the sign of $(T_e\text{-}T)$, C_4 is a constant, and Q_t is the activation energy for the transformation.

This model aggress well with the kinetic data available, predicts a hysteresis in the transformation on heating and cooling, a typical "c" shaped time-temperature-transformation curve on cooling with the "nose" at approximately the right temperature[30], and that the transformation is suppressed at high cooling rates in agreement with the occurrence of a martensitic for cooling rates >40-600 $K.s^{-1}$[27].

3-8. Transformation Hardening

As Zr passes through the α-to-β phase transformation in either direction, it undergoes a shear strain equivalent to an extension of about 10%, although, without an applied stress this shear is randomly oriented because of the symmetry of the bcc crystal structure, and does not produce a macroscopic strain. A dislocation structure is generated which causes a cooling rate dependent hardening, resulting in inverted primary creep of the β-phase after heating [15], and "quench hardening" of the α-phase on cooling [31,32]. Sills and Holt [17] estimated this effect by equating the "transformation strain rate", $\dot{\varepsilon}_0$, to the strain rate due to dislocation creep given in section 3-1, i.e.,

$$\dot{\varepsilon}_0 = \left|0.1\dot{f}_\alpha\right| = C_j \exp\left(-Q_{j1} / TR\right)\sigma_*^k$$

which allowed them to calculate the evolution of σ_I according to

$$\dot{\sigma}_i = \partial\sigma_i / \partial t = U_j E_j \dot{\varepsilon}_0 / \sigma_i^p - B_j / T\sigma_i^q \sigma_*^h \exp\left(-Q_{j2} / RT\right)$$

for both the β-phase on heating and the α-phase on cooling. This equation gave good agreement with experimental quench hardening data for the α-phase.

3-9. Subsequent Developments.

The combination of models described in Sections 3-1 to 3-8 (with the exception of the dynamic phase transformation model) was able to reproduce "ballooning tests" in an inert environment [33,34] very well and able to give a reasonable semi-quantitative representation of important effects in such tests of initial metallurgical condition of the fuel cladding associated with braze heat-affected zones [35,36]. The models were embodied in the computer code NIRVANA [37].

Subsequently, the Sagat, Sills and Wadsworth [36] extended the model to include the effects of oxidation on the deformation of the alpha phase, based again on data obtained at McGill University under contract to AECL [38,39], the kinetics of the phase transformation and the effect of the oxide on the external surface of the cladding based on AECL's in-house data [36]. These modifications were incorporated into NIRVANA which is still in use.

4. Predictions.

An interesting qualitative prediction of the model is that, with a very rapid power insertion, the expansion of the fuel could out-pace the annealing of radiation damage in the cladding, resulting in localized strain and failure similar to that hypothesized under power ramp conditions during normal operation, see Section 2. Such failures were observed in US DOE tests [40,41]. NIRVANA contains a flag to warn the user of this possibility when the predicted plastic strain exceeds a set threshold at a high strain rate before complete annealing of the damage has taken place. This flag was activated art least once during studies of the Bruce power pulse transient in the 1990s.

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