Modeling Irradiation Creep and Growth with VPSC

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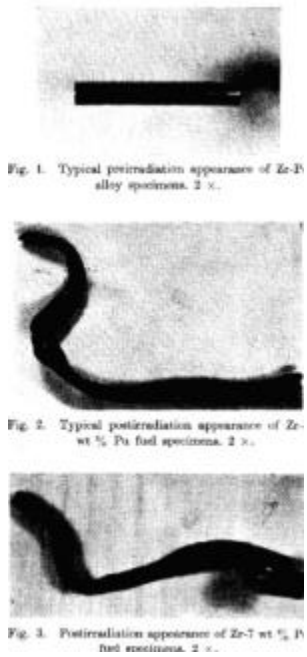
During service in a commercial power reactor, the components are subjected to high heat and pressure, and bombarded by radiation. The combination of these stressors causes most materials to deform elastically and plastically over time. For zirconium-based alloys, thermal creep, irradiation creep, and irradiation growth are the primary modes of deformation.



Experiments in the '60s noted irradiation creep and growth effects [Horak, Rhud, J. Nucl. Mater. 3 (1961)]

The driving force for thermal creep is high temperature; temperatures greater than approximately 30% of the melting temperature produce high diffusivities of vacancies and interstitials, allowing for their preferential absorption by dislocations.

In reactor environments, the neutron bombardment produces a large number of vacancies and interstitials (point-defects). The accumulation of point-defects, known as "sinks," attracts other defects where they recombine and become trapped. In the absence of an applied stress, dislocations present in the lattice preferentially absorb the defects, causing them to climb, and this phenomenon is known as irradiation growth. Irradiation also produces clusters of mobile self-interstitial atoms (SIAs). The SIA clusters are assumed to interact only with dislocations and dislocation loops with the same Burgers vector; consequently, they are the driving force of the anisotropy of irradiation growth.

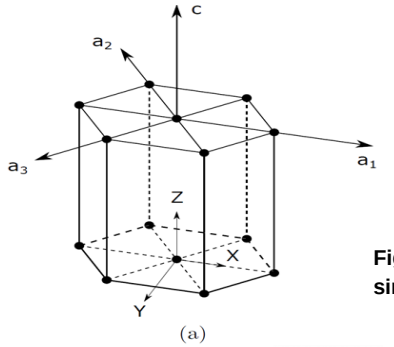


Figure 7 Illustration of a single crystal of Zircaloy

When a resolved shear stress is present, the dislocations climb *and* glide, and this phenomenon is known as irradiation creep. Irradiation creep can be induced by irradiation growth: the growth of a grain is opposed by interaction with its neighbors and the resulting stresses induce irradiation creep.

CASL will incorporate a science-based model known as visco-plastic self-consistent (VPSC) to predict irradiation growth and creep. The VPSC approach is a means to predict the macroscopic response of a polycrystalline aggregate, assuming knowledge of the constitutive law of a single grain. VPSC treats each grain as an inhomogeneity included in an effective medium, and iteratively solves for the response of the macroscopic effective medium. LANL and ORNL researchers have incorporated a VPSC crystallographic model of grains and interfaces into a code and are studying the atomistic mechanisms contributing to creep and growth.

The constitutive response of the single grain illustrated in Figure 7 due to creep and growth in its simplest form is:

$$\dot{\varepsilon}_{ij}^{g} = \dot{\varepsilon}_{ij}^{\text{creep}} + \dot{\varepsilon}_{ij}^{\text{growth}}$$

The creep rate for the three types of slip systems (prismatic, basal, and pyramidal) is a function of neutron flux, dislocation density, and applied stress is:

$$\dot{\varepsilon}_{ij}^{\text{creep}} = \sum_{s} m_{ij}\dot{\gamma}^{s} = \dot{\gamma}_0 \sum_{s} m_{ij}^{s}(m_{kl}^{s}\sigma_{kl}^{s})K^{s}\left(\frac{\rho^{s}}{\rho_{\text{ref}}}\right)\left(\frac{\phi}{\phi_{\text{ref}}}\right) = M_{ijkl}^{g}\sigma_{kl}^{g}$$

where $\dot{\gamma}^{s}$ is the dislocation density and Φ is the neutron flux . The creep rate equation can be transformed to provide the strain rate tensor and resolved shear stress on the system and represents a linear dependence of creep rate with stress, dislocation density and neutron flux.

The creep compliances for each type of dislocation mode, reflecting the most effective creep mechanisms, are:

$$K_{prism} = 10.57\ MPa^{-1};\ K_{basal} = 4.14\ MPa^{-1};\ K_{pyramidal} = 0.11\ MPa^{-1}$$

K can also be regarded as the inverse of a characteristic resistance for moving each type of dislocation. The creep compliances were fit to experimental irradiation creep of Zr-Nb tubes, assuming a constant growth rate for every crystal.

Since irradiation creep is associated with dislocation trapping of irradiation-produced defects, it is expected to increase monotonically with dislocation density and with the number of defects being produced per unit time. The production of defects such as prismatic and basal loops is provided by experimental information as a function of irradiation dose.

To test the model, a single crystal was evaluated with the crystallographic axes aligned with the coordinate axes (see Fig. 7). Fig. 8 (top) shows the normal strain in all three directions as a function of irradiation dose as predicted by the model. The results compare well with empirical results for a single Zircaloy-4 crystal (Fig. 8, bottom). As expected, the irradiation growth model predicts the shrinkage of the crystal along the c-direction, and expansion along the a-directions. The team also investigated the response of textured materials, including rolled Zircaloy-2 and a random texture, both illustrated in Fig. 9. The results, plotted in Fig.10 and 11, are as expected.

Additional modeling is focused on measuring the interaction energy of point-defects with dislocations. The interaction energy is a direct measure of favorability for defect-dislocation interaction. Nine different types of point-defects can be identified in HCP Zirconium. These are listed in Table 1, along with

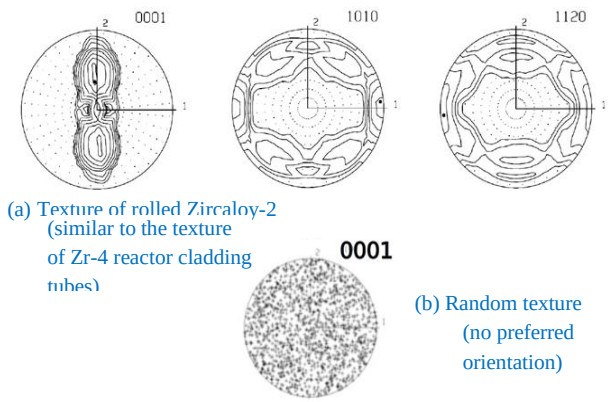


Figure 9 Pole figures of polycrystal aggregates

their formation energies as identified by the application of the VPSC study and compared with a previous study. The behavior of interstitials in a strain field and related diffusion energy barriers were also studied.

For more information, see *Atomistically informed model of thermal and irradiation creep in Zirconium,* CASL, 10/3/2011 (G. Subramanian et. al.); *Progress report on the incorporation of lower length scales into polycrystal plasticity models,* CASL, 10/15/2012 (G. Subramanian & C. Tome); LA-UR-12-25612.

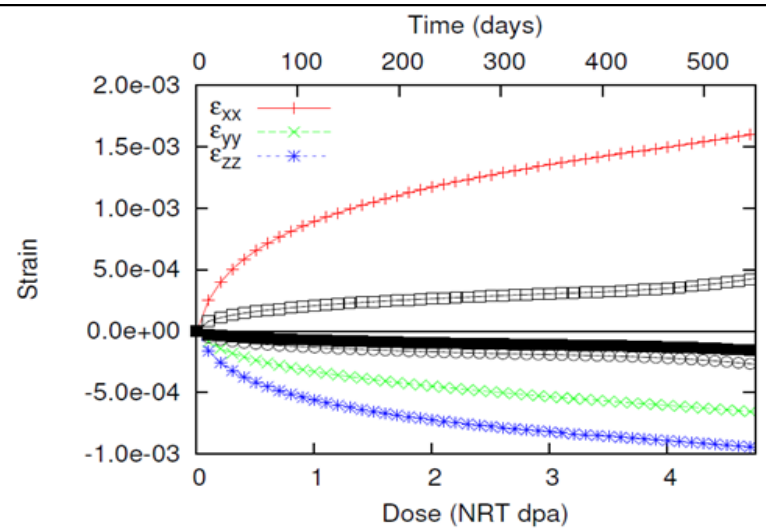


Figure 11 Predicted response of polycrystal with rolled texture, with increased dislocation density. Black symbols are data from Fig. 8.

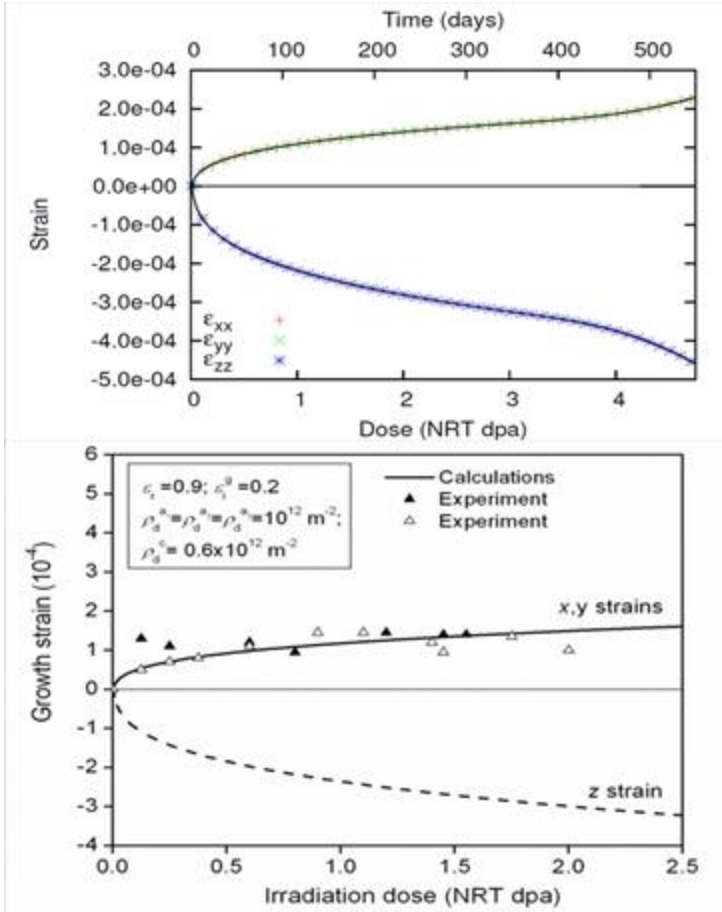


Figure 8 The VPSC-Irradiation growth (top) and experimental measurements on single crystal Zircaloy-4 (G.J.C. Carpenter, R.A. Murgatroyd, A. Rogerson, and J.F. Watters, Journal of Nuclear Materials, 101:28, 1981)

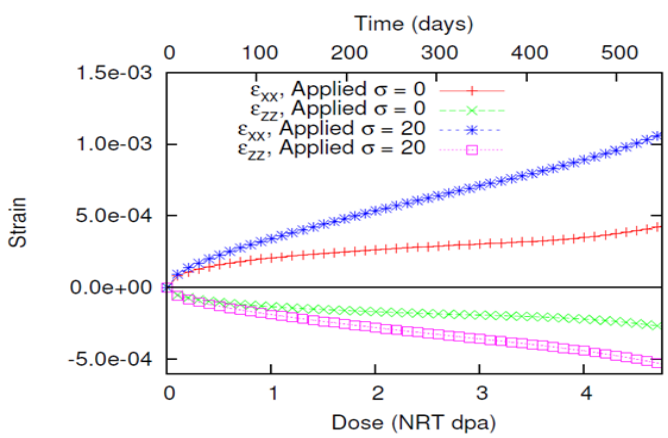


Figure 10 Effect of externally loading the textured polycrystal. Since the load opposes the direction of growth of the polycrystal, the strains in the loaded polycrystal are lesser than the unloaded polycrystal.

Table 1: Various types of point defects in α-Zirconium, and their formation energies [GGA DFT data: F. Willaime, J Nucl. Matls, 323:205, 2003]

Defect Type	Formation Energy (eV) This study	GGA DFT [14]
Basal Crowdion (BC)	2.876	–
Basal Octahedral (BO)	2.897	3.14
Basal Split (BS)	2.878	3.39
Basal Tetrahedral (BT)	–	–
Crowdion (C)	3.135	3.52
Octahedral (O)	2.882	3.04
Split (S)	2.779	3.28
Tetrahedral (T)	–	–
Vacancy (V)	1.688	??