Methods for Integrating Micro-scale Creep modeling into Finite Element Simulations of Fuel Rods

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One of the fundamental challenges of multi-scale modeling is the integration of atomistic-scale effects to continuum scale calculations. For example, the analysis of creep deformation requires continuum-level finite-element calculations to compute local stresses and temperatures which are then used in atomistic models to determine local atom and dislocation response, which feed back to the overall creep response. Due to the complexities involved, different types of analytical approaches are needed at different scales, and establishing a framework where models from different scales are incorporated at the other scales can be a difficult task.

For example, even a numerical look-up table runs into considerable numerical difficulty considering the number of dimensions that such a table needs to be useful. Also, empirical approaches to creep models may obscure insights to the physics mechanism and they cannot be used to extrapolate to new design spaces. As an alternative, the concept of creep-mechanism maps can allow multiple dominant creep mechanisms to be identified and applied in different parts of a component, depending on the local stress state and temperature, and also allows these to change as the local conditions change.

The mechanisms of steady-state creep that are valid when there is no microstructural evolution are diffusional creep (in which atoms diffuse in response to a stress gradient), dislocation glide (in which flow is controlled by the motion of dislocations), and dislocation climb (in which thermal energy provides an additional mechanism for dislocations to overcome obstacles). Each of these laws has a characteristic constitutive relationship between stress and strain rate that can be incorporated into finite-element models.

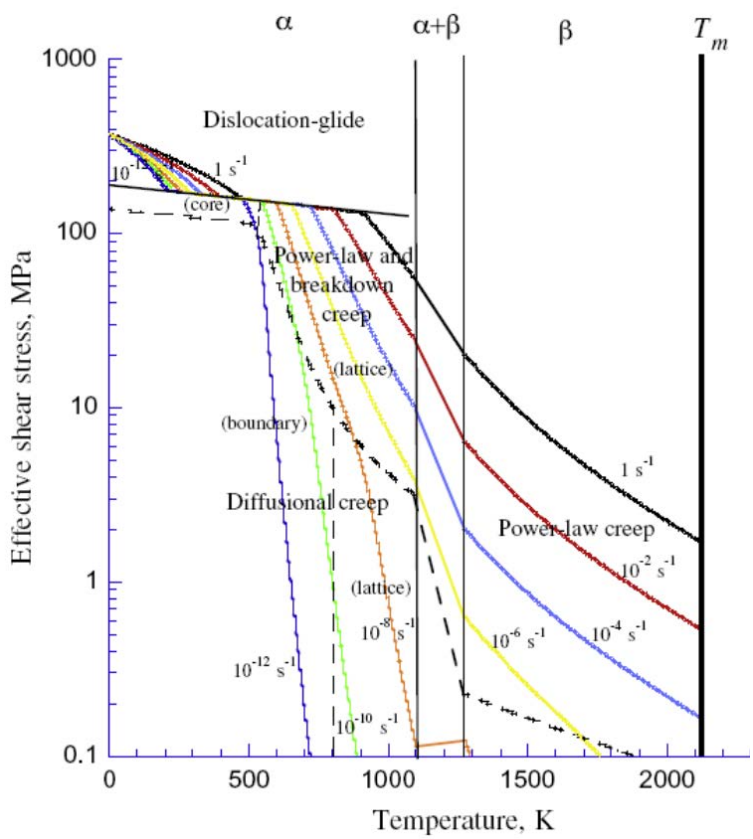

Figure 14 A deformation-mechanism map drawn using the equations developed for unirradiated Zircaloy-4 with a grain size of 150μm

A creep-mechanism map is drawn as contours of constant strain rate in a stress–temperature space, as shown in Figure 14. In general, all mechanisms are assumed to act simultaneously, and the boundaries between the different mechanisms are drawn when the dominant mechanisms switch.

As a demonstration of the effectiveness of the creep-mechanism map approach, the constitutive equations associated with each of the dominant mechanisms were implemented within a commercial finite element package (ABAQUS). A Zircaloy-4 tube (thickness 0.024") was modeled as bonded to a cylinder of UO_2 fuel (0.315" diameter) with a semicircular chip in it (0.010" depth) as shown in Fig. 16. The equations for the creep mechanisms of UO_2 were taken directly from Frost and Ashby[2]; the various creep mechanism models for the Zircaloy-4 were taken from a variety of sources,[3] and incorporated into the finite-element code as a creep-mechanism map. The actual creep rate at any point is determined by adding the rates from all the mechanisms that contribute simultaneously and by selecting the fastest of the mutually exclusive mechanisms. The advantage of this approach is that no a priori assumption about the creep law needs to be built into the FEM code. It is determined on the fly while the calculations proceed. This means that different portions of a structure can exhibit different creep mechanisms, depending on the local stress and temperature. Furthermore the same portion of a structure can exhibit different mechanisms with time, as the stress and the temperature evolve.

The effects of radiation, such as swelling, growth and microstructural changes were not included for either the fuel or cladding for the demonstration, but could be incorporated just as easily if the supporting data exists. The steady-state temperature profile shown in Fig. 16 was developed by applying a power density of 95 MW/m^3 to the fuel and fixing the clad surface temperature at 550 K. This steady-state temperature profile was then imported into a 2-D plane-strain finite-element model to calculate the stresses and the creep rates using the creep-mechanism map for the

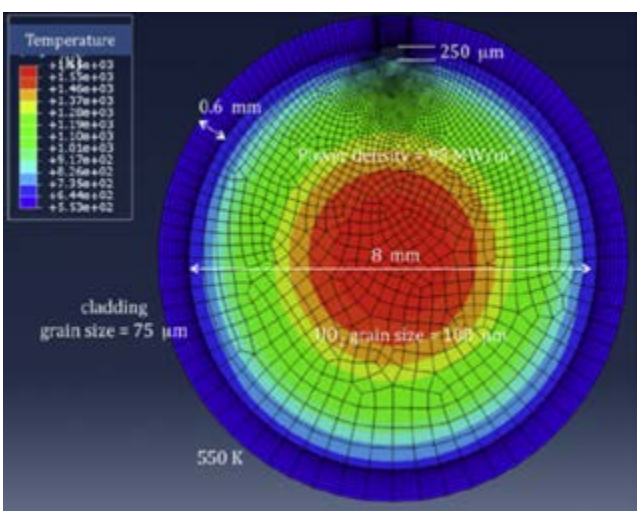

Figure 16 Steady state temperature profile for the cladding and fuel pellet configuration studied

Zircaloy and the fuel. The evolution of the deformation mechanisms with time is shown in Fig. 17.

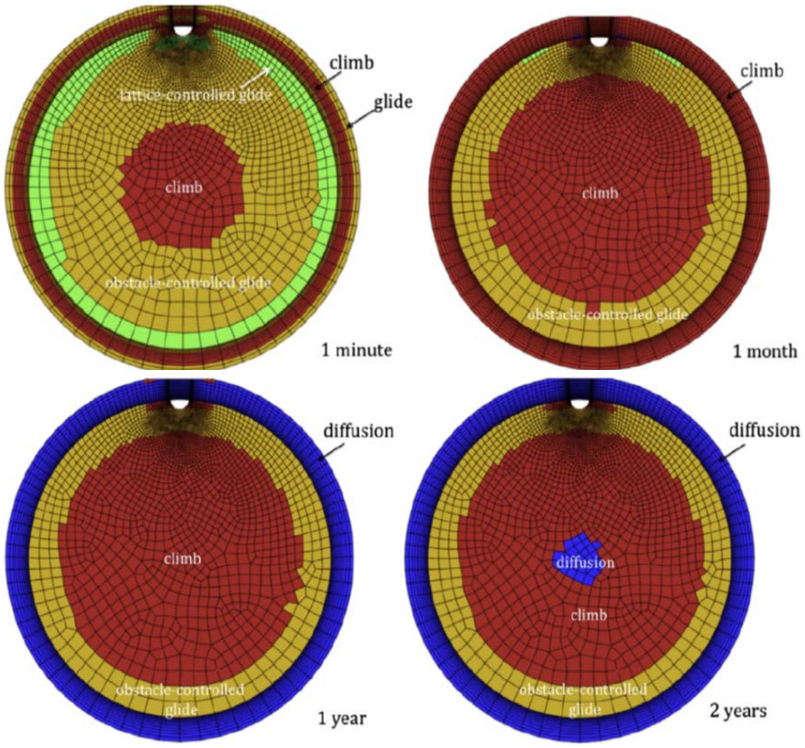

Figure 17 Evolution of deformation mechanisms with time for the cladding and fuel assembly studied

While deformation maps were first conceived and developed more than 30 years ago, they didn't become easy to implement until modern computing capabilities were made available. The frame-work allows the constitutive creep equations appropriate for a particular temperature and stress state to be automatically invoked during a creep analysis. To realize an ultimate goal of multi-scale modeling of a commercial power reactor, additional models need to be developed that link the effects of radiation to creep, including radiation growth, radiation creep, and changes in microstructure.

It is likely that this approach can be applied to many multi-scale, multi-physics problems. For example, in the problem of grid-to-rod fretting, different creep mechanisms are needed to calculate deformation of the cladding and relaxation of the contact stresses between the grid and the cladding. An accurate prediction of the changes in geometry and evolution of the contact stresses require an accurate creep model that can efficiently apply the effects of temperature and stress, in addition to radiation effects.