Numerical Simulation of Fuel Microstructural Evolution in a Thermal Gradient

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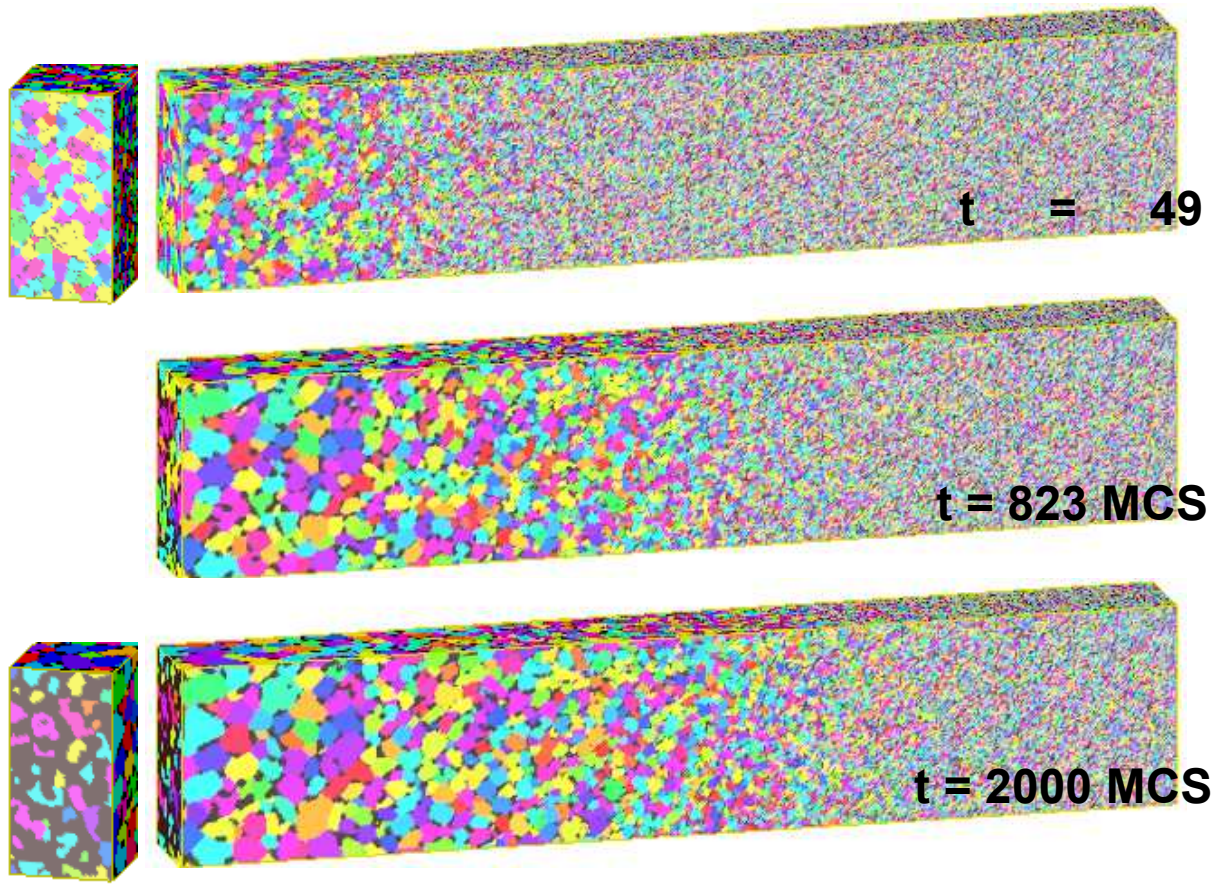
A key feature of virtually all nuclear fuels, including fast reactor fuels, is the large temperature gradient that fuel pellets experience during normal operation. These large temperature gradients drive a number of microstructure evolution processes that are unique to the nuclear fuels and particularly to fast reactor fuels. Among them is the non-homogeneous diffusive processes. In this work, we focus on grain growth coupled to void and gas bubble migration in such a large temperature gradient. A discrete statitstical-mechanical model, the Potts kinetic Monte Carlo model will be used to munerically simulate microstructural evolution at the mesoscale. The Potts model has been developed over two decades to study many microstructural evolution processes including normal and abnormal grain growth, Ostwald ripening, grain growth in the presence of mobile and immobile pinning phase and sintering The processes of interest in this work are grain growth and bubble migration in large temperature gradients. Previous work has developed 2D[i] and 3D[ii] grain growth in temperature gradients as well as grain growth coupled with void migration in a 2D polycrystalline[iii] and 3D idealized polycrystalline[iv]. In this work,we extend the the 3D grain growth and bubble migration to the general case of a 3D polycrystalline material such as that of nuclear fuels.

Potts kinetic Monte Carlo Model

The model used here to simulate the microstructural evolution of a full 3D digitized microstructure has been described in detail elsewhere. Curvature driven grain growth, bubble migration by surface surface in a temperature gradient has been simulated by varying the grain boundary mobility and surface diffusivity as a function of temperature. A heat of transport term as described in the diffusion literature has been added to the simulate the net transport of the gas towards the high-temperature side.

Simulation Results

The resulting microstructural evolution of grain growth and bubble migration is shown in FIG 1. The colored features are grains; the black features are bubbles. The starting microstructure is a homogeneous polycrystalline material with small isolated bubbles (in case of fresh fuel the bubbles are pores due to incomplete sintering) evenly distributed in the fuel. A temperature gradient is applied across the material with the high-temperature at the left side and the low-temperature at the right side. As the results show, both the grains and bubbles coarsen at a much higher rate at the high-temperature side due to higher bubble diffusivity and grain boundary mobility at the high-temperatures. The rate controlling process is the coarsening of bubbles, which pin the grain. As the bubble coarsen by coalescence, they unpin the grains locally and allow a burst of grain growth. Simultaneously, there is a net flux of the



bubbles towards the high-temperature side as shown in the side view at the left side. Early in the simulation at time t = 49 MCS, the bubbles are homogeneously distributed through out the sample. However, at time t = 2000 MCS, the bubbles are diffusing toward the high-temperature side. The bubbles have become large and connected and grains are poking into the bubbles.

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References

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