Numerical Modeling of Gaseous Fission Product Transport at the Meso-scale: A Multi-physics Approach for Fuel Pin Swelling – FR09P1379

SAND2010-4808C

T. J. Bartel*(tjbarte@sandia.gov), L. N. Brewer*, R. Dingreville**, M. T. Lusk***, J. Robbins*, T. Semi***, L. Zhang** .

*Sandia National Labs, USA; **New York University-Polytechnic, USA; ***Colorado School of Mines, USA

Introduction

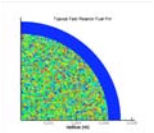
Goal:

Develop a validated and predictive capability to simulate the mechanical response of a fuel pin during a rapid transient thermal event at the meso- to continuum scale using fundamental physics models.

→**that is, to predict fuel pin clad strain during a rapid thermal transient**

Physics Requirements:

- rapid thermal transient
  - time accurate
- function of burn-up
  - fission gas inventory and location
    - intra- and inter- grain
  - mechanical response of polycrystalline materials
    - viscoelastic & viscoplastic constitute models for fuel & clad
  - grain restructuring
  - gas transport during transient thermal conditions
    - atomic, clusters and bubbles



Geometry Requirements:

- 3D
  - radial cross-section (2D) plus small axial dimension (Z)
  - assume 10 micron diameter grains, 5 mm diameter fuel pin
    - ¼ pin cross-section ~ 62,000 grains
    - assume dZ = 100 grains, then computational domain => order 6.2 M grains

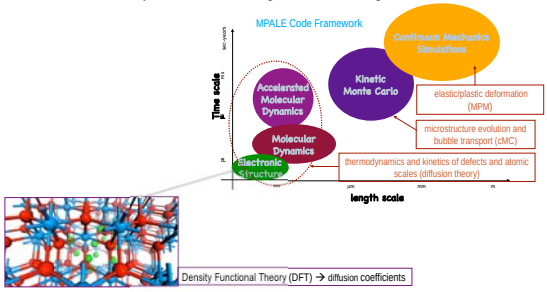
Computational Requirements:

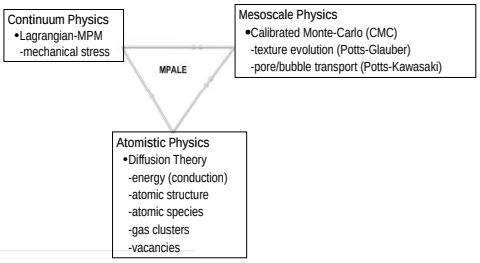
- massively parallel computer

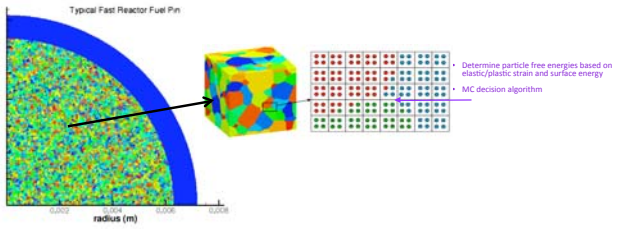
Method

3D Computational Code: MPALE

- directly couple phenomena at micro-scale and continuum scale (sub-grain to fuel pin)
- time split algorithm: material wave speed much higher than material transport or grain evolution
- lower length scale information computed with DFT and upscaled via diffusion models
- particle & cell based continuum mechanics algorithm (material point method)
- calibrated Monte-Carlo particle method for grain restructuring



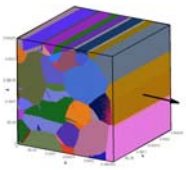


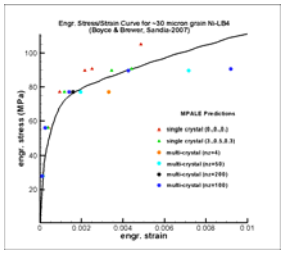


Results

Continuum Mechanics

- validation of polycrystal elasticity and plasticity
  - comparison with nickel tensile test
    - grain morphology from EBSD (2D data set)
    - 60 different Euler angle combinations



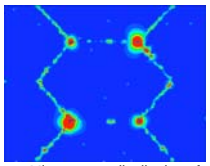


- current work: non-local plasticity and viscoelastic constitutive models for UO_2

Mesoscale Physics

- time calibrated Potts based algorithm (cMC) has been developed and validated
  - 1 MCS => physical time step!
  - required to couple MC algorithm with continuum mechanics
- Potts-Kawasaki for bubble transport
  - example: pressurize bubble (ideal gas) from transient thermal condition

bubbles collect along grain boundaries



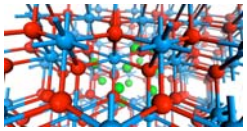
von Mises stress distribution after thermal transient

Atomistic Physics

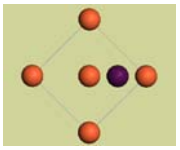
- assume diffusion theory for transport
- issue: determine diffusion coefficients for actinides
  - function of temperature and strain (lattice spacing)
- strategy: use DFT to determine relative trends in diffusion coefficients
  - DFT functionals for actinides are not mature; uncertainity in absolute value of D is too large

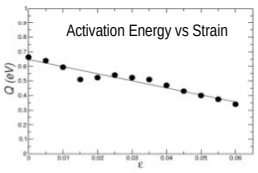
activation energy for diffusion

$$D = D_0 \exp\left(-\frac{Q}{kT}\right)$$



- simulate vacancy transport in Cu to demonstrate strategy





from Crosby-2003

Future Work

- Implement implicit time integration scheme to replace explicit scheme in MPALE
- Implement parallel non-local plasticity and viscoelastic constitutent model
- Determine equivalent MC time calibration for Potts-Kawasaki
- Determine diffusion coefficient trends for UO_2 using DFT
- Investigate and implement material damage models for fuel and clad
- Validate with potential transient strain validation experiments @ SNL ACCR

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.