Multiscale modeling of fission gas behavior for BISON

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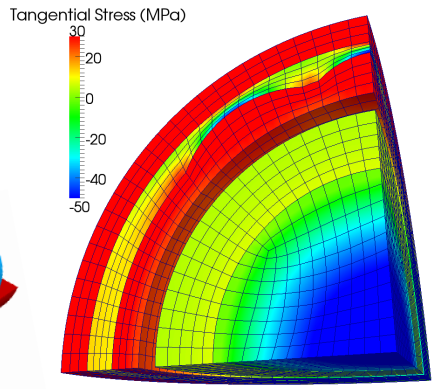
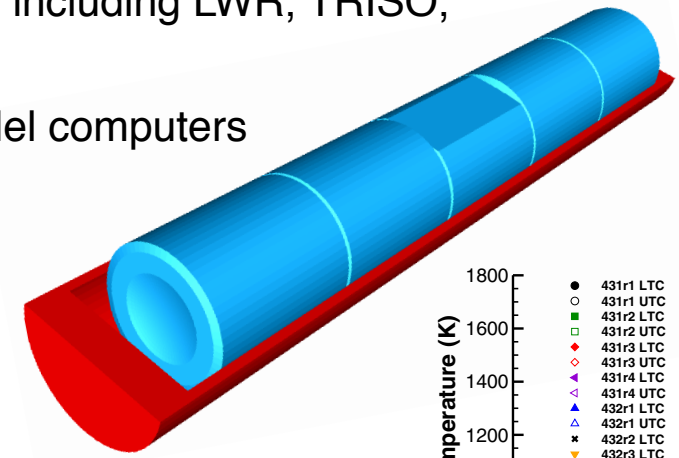
Outline

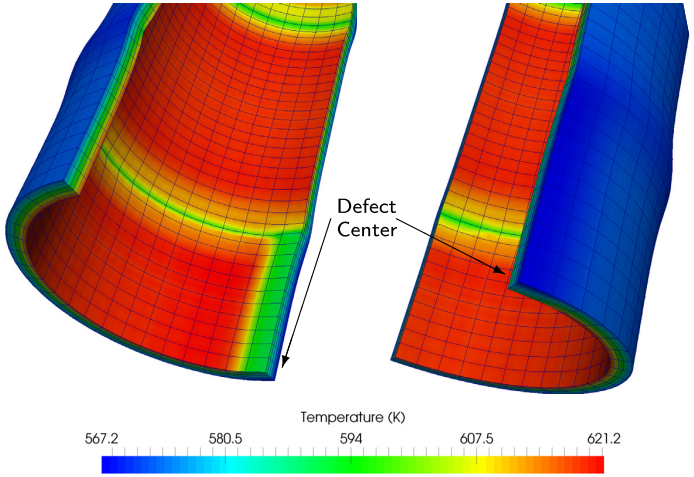
- BISON fuel performance code
- Fission gas model for UO_2
- Examples of validation results
- Lower-length scale modeling for the parameters
- Multiscale fission gas model for U_3Si_2
- Outlook
- Acknowledgements

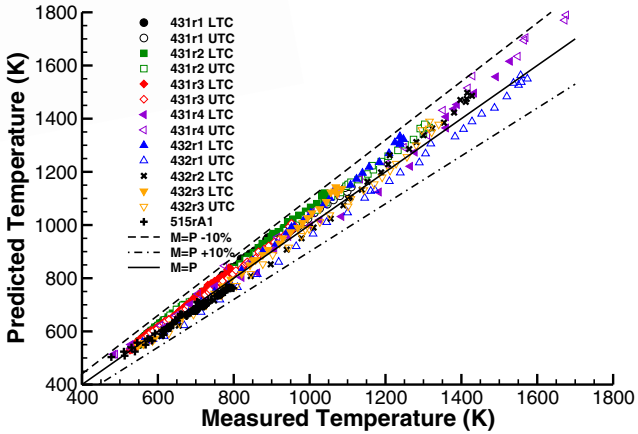
BISON fuel performance code

- Finite element based, engineering fuel performance code based on INL's open-source MOOSE framework
- Solution of fully-coupled equations of thermo-mechanics in 1D, 2D, or full 3D
- Used to analyze various fuel forms including LWR, TRISO, and fast metal and oxide fuels
- Designed for efficient use on parallel computers



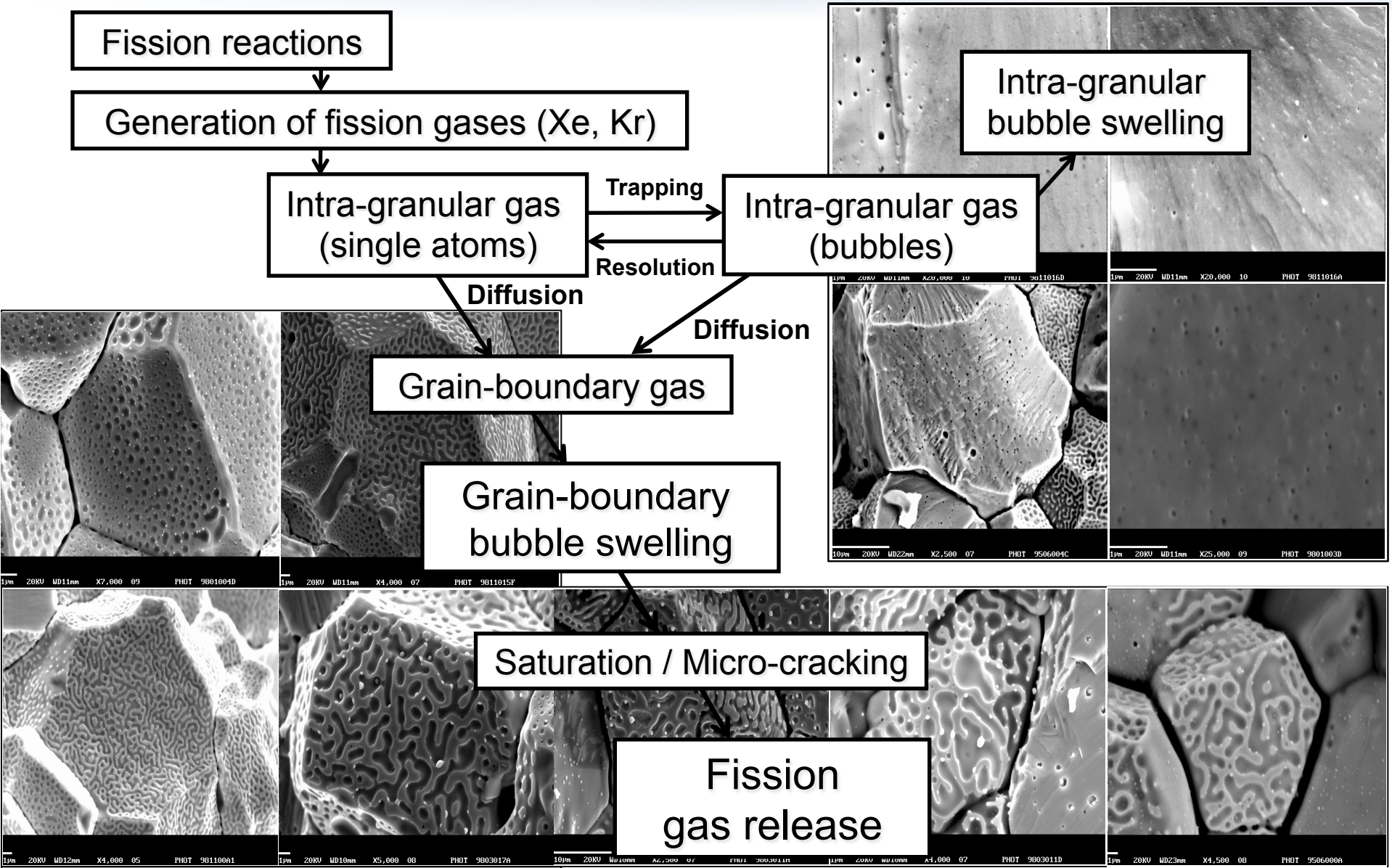






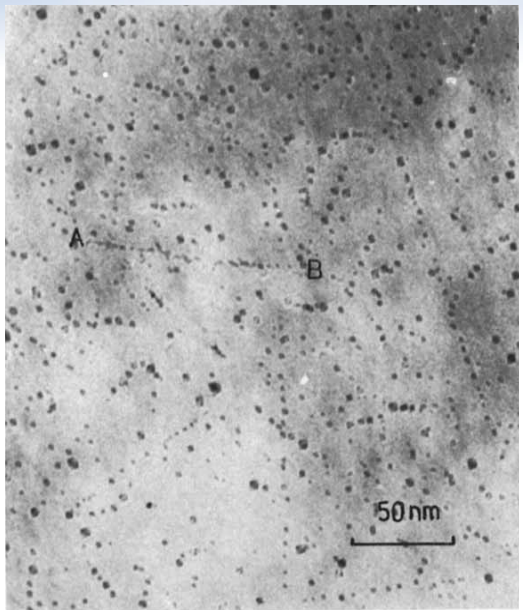
R.L. Williamson et al., Multidimensional multiphysics simulation of nuclear fuel behavior, J. Nucl. Mater. 423, 149, 2012
J.D. Hales et al., Multidimensional multiphysics simulation of TRISO particle fuel, J. Nucl. Mater. 443, 531, 2013
B.W. Spencer et al., 3D modeling of missing pellet surface defects in BWR fuel, Nucl. Eng. Des. 307, 155, 2016
R.L. Williamson et al., Validating the BISON fuel performance code to integral LWR experiments, J. Nucl. Mater. 301, 232, 2016

Stages of fission gas behavior



Intra-granular model

- Computes intra-granular bubble evolution and swelling, and gas diffusion to grain boundaries
- Derived from cluster dynamics equations, simplified for application to engineering codes
- Can be informed with improved parameters from advanced lower-length scale models

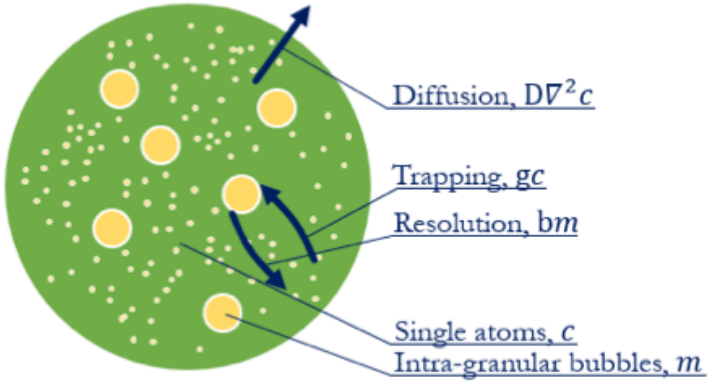


C. Baker, J. Nucl. Mater. 66, 283-291, 1977

$$\frac{\partial N}{\partial t} = +\nu - \alpha_{\bar{n}} N$$

$$\frac{\partial m}{\partial t} = +2\nu + \beta_{\bar{n}} N - \alpha_{\bar{n}} m$$

$$\frac{\partial c_1}{\partial t} = +yF + D\nabla^2 c_1 - 2\nu - \beta_{\bar{n}} N + \alpha_{\bar{n}} m$$



Grain-boundary model

- Bubble growth with inflow of atoms and vacancies (*Speight and Beere, Met. Sci. 9, 1975*)

$$\frac{dn_v}{dt} = \frac{2\pi D_v \delta_g}{kTs}\left(p - p_{eq}\right)$$

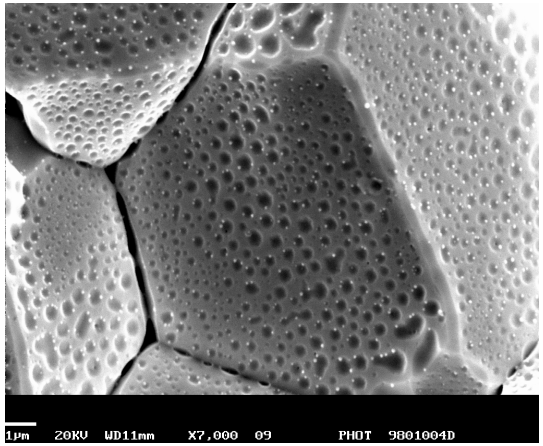
- Bubble coalescence with geometrical reasoning *(White, JNM 325, 61-77, 2004)*

- Gaseous swelling coupled to FGR

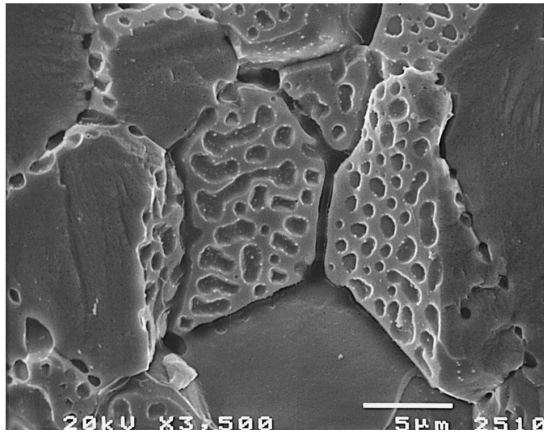
- Two FGR contributions:
  - Grain-boundary saturation

$$\frac{dF_c}{dt} = \frac{d(N_{gf}A_{gf})}{dt} = 0 \qquad if\ F_c = F_{c,sat}$$

  - Burst release associated with micro-cracking

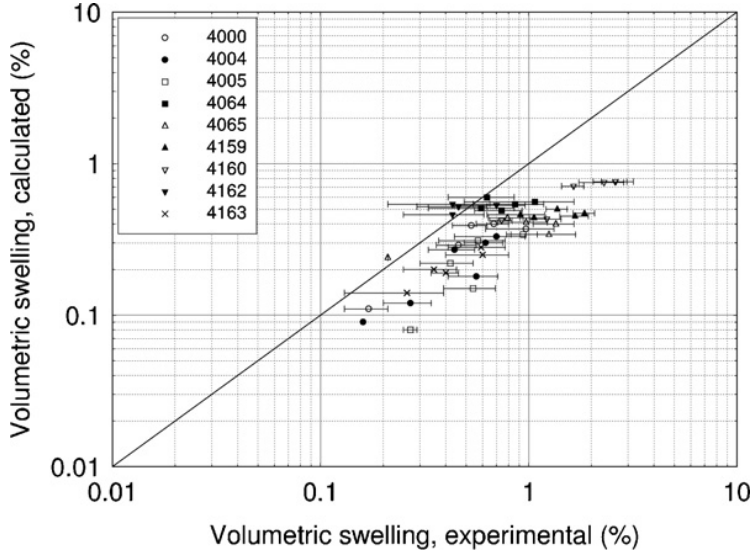


R.J. White et al., Tech. Rep. R&T/NG/EXT/REP/0206/02, 2006

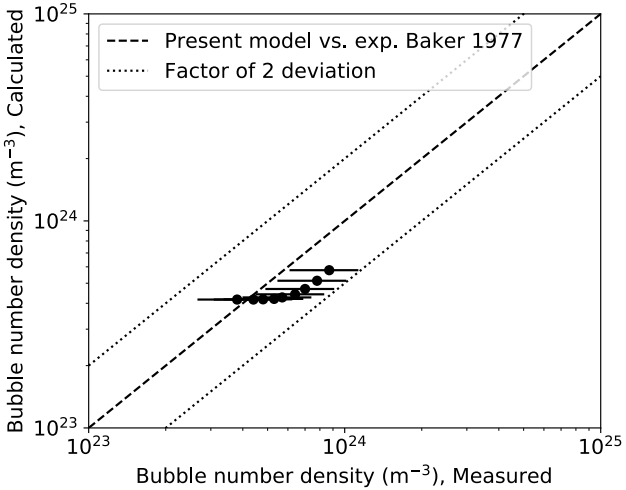


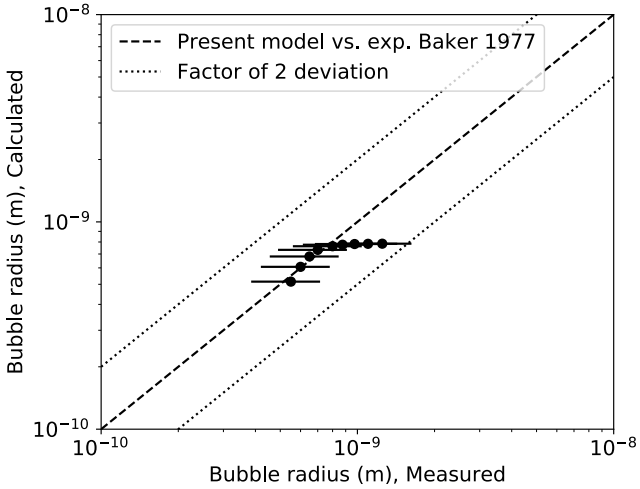
I. Zacharie et al., J. Nucl. Mater. 255, 85, 1998

Separate-effects validation examples



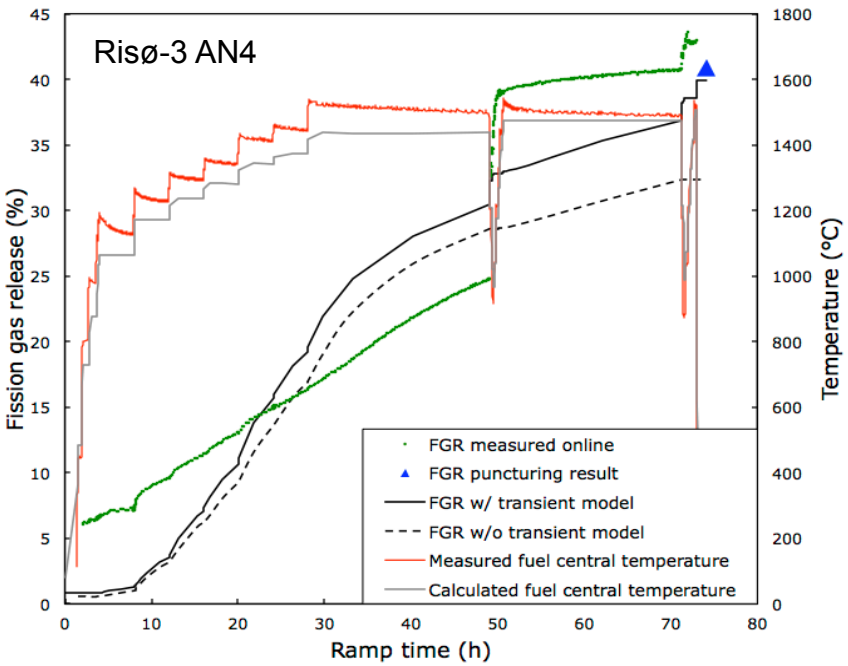
Comparisons of local grain-boundary swelling in power-ramped UO_2 (Pastore et al., NED 256, 2013). Experimental data from White et al., R&T/NG/EXT/REP/0206/02, 2006.



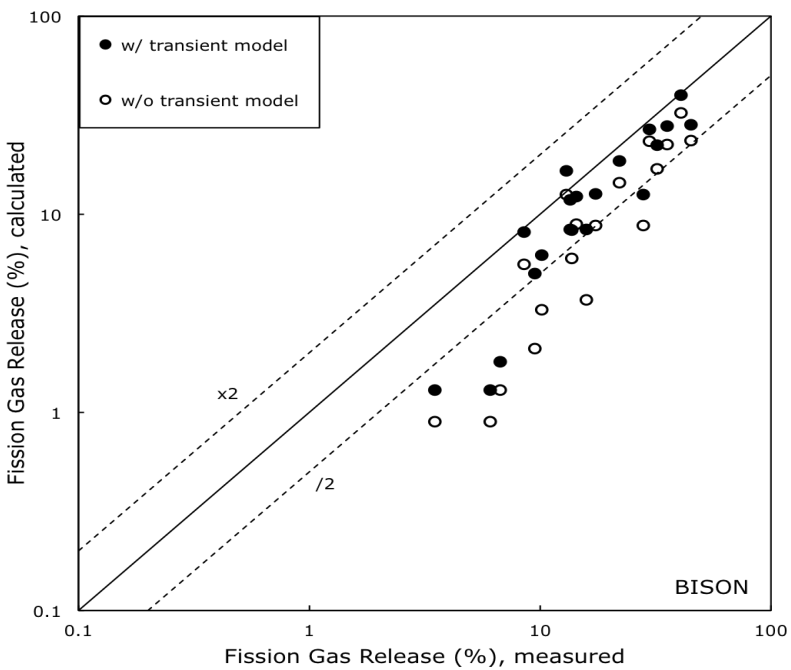


Comparisons of local intra-granular bubble number density and size in base-irradiated UO_2 (Pizzocri et al., JNM 502, 2018). Experimental data from Baker, JNM 66, 1977.

Integral validation examples

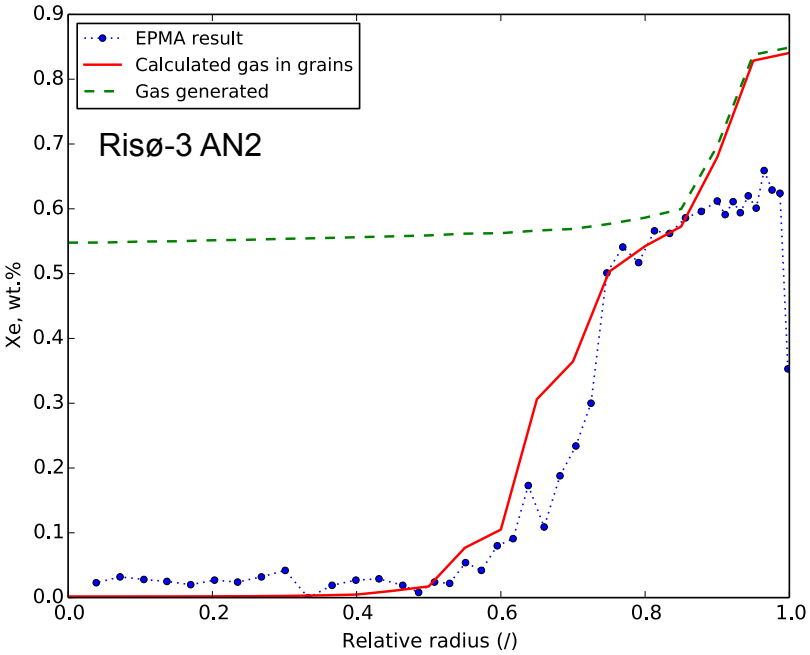


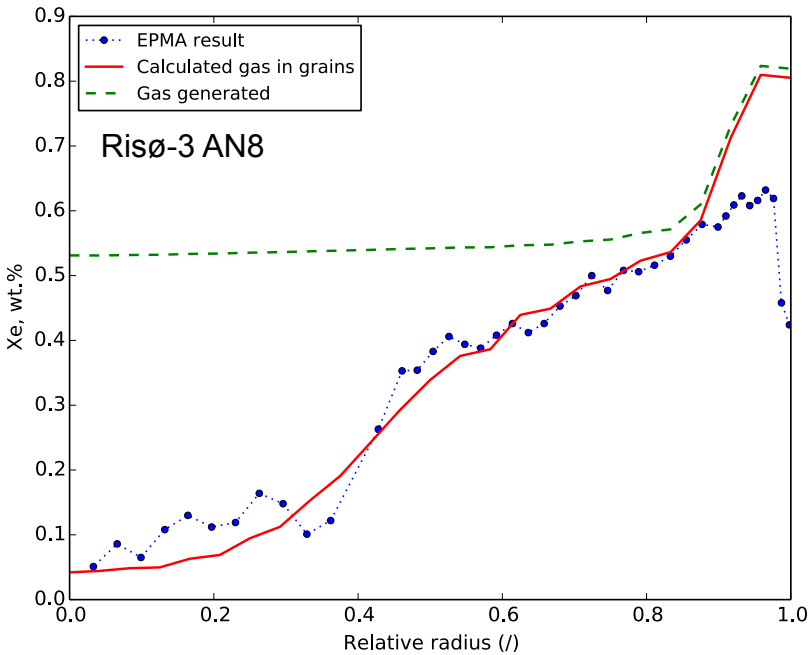
Integral FGR vs time during LWR fuel rod power ramp experiment (Risø-3 AN4)



Integral FGR at EOL for 19 LWR fuel rod power ramp experiments

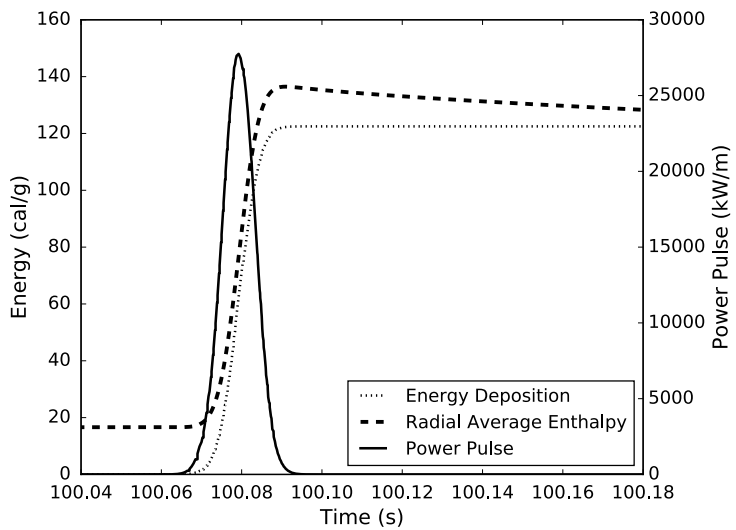
Integral validation examples

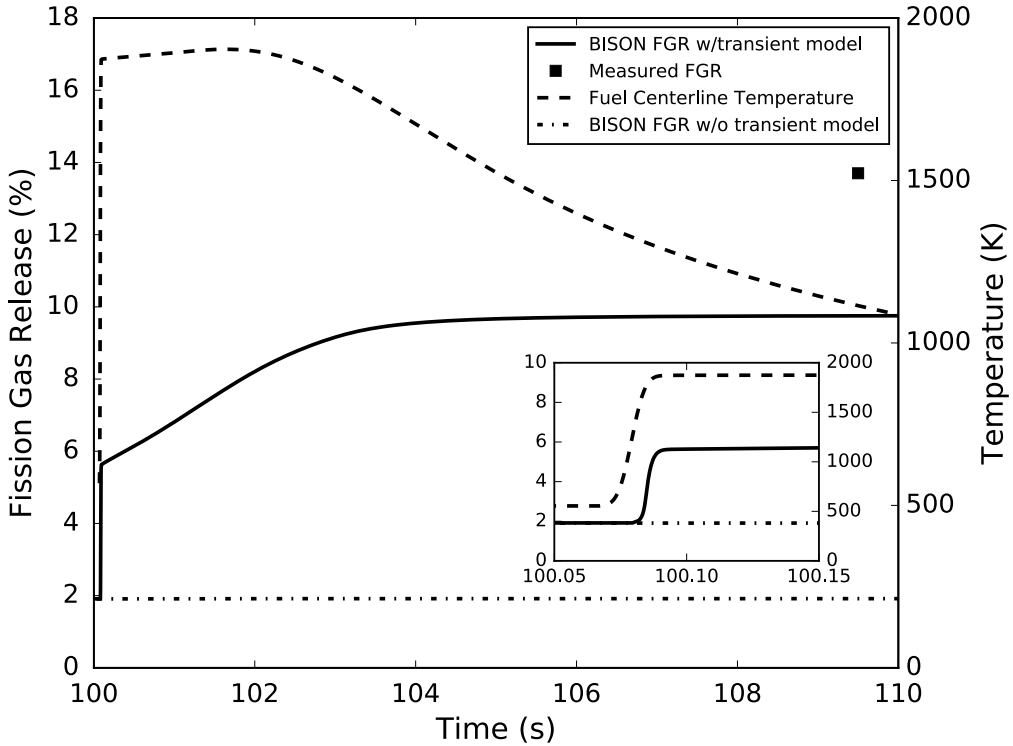




Radial profiles of Xe concentration after ramp tests calculated with BISON and PIE data

RIA integral simulation example

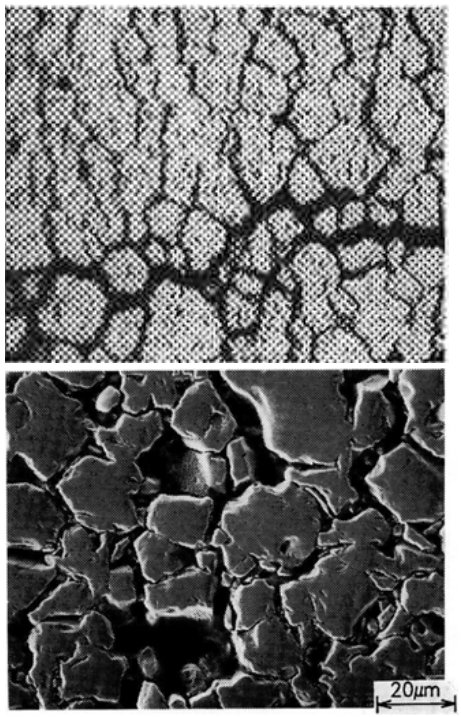


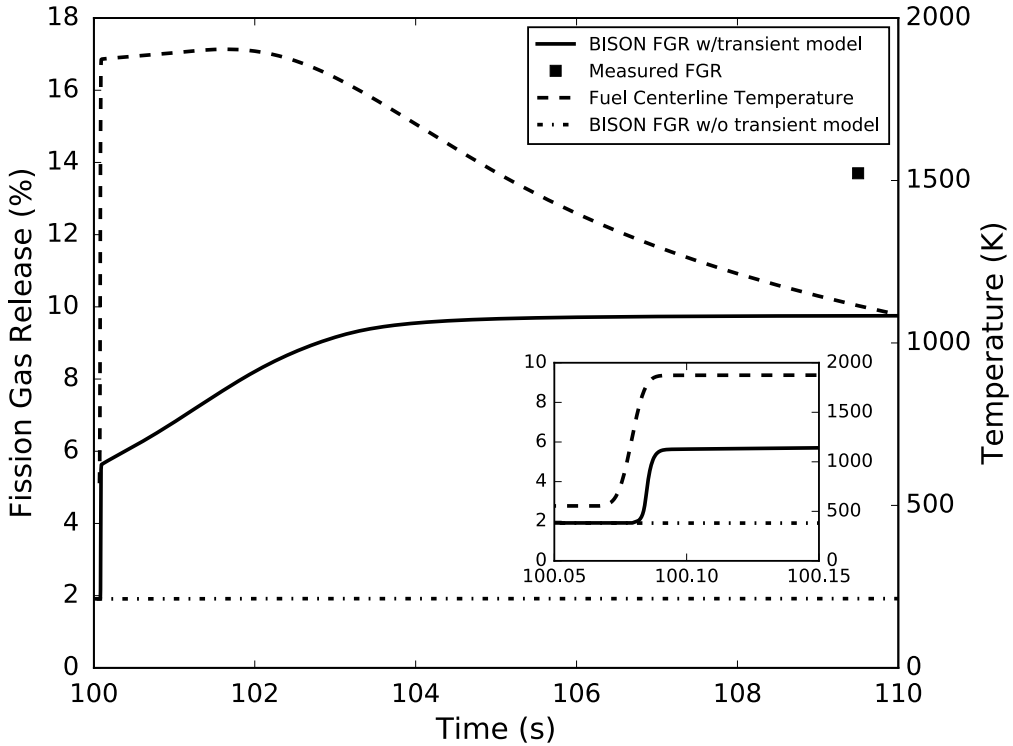


CABRI REP Na-3 power pulse test

Left: Power, calculated energy deposited and radially averaged fuel enthalpy at peak power node
Right: FGR with fuel centerline temperature. The inset shows a shorter time around the power pulse

RIA integral simulation example





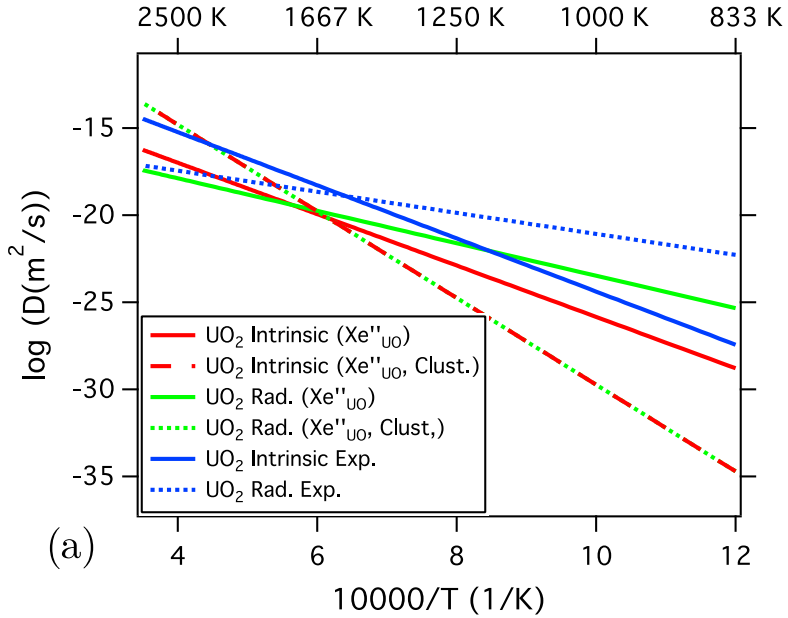
CABRI REP Na-3 power pulse test

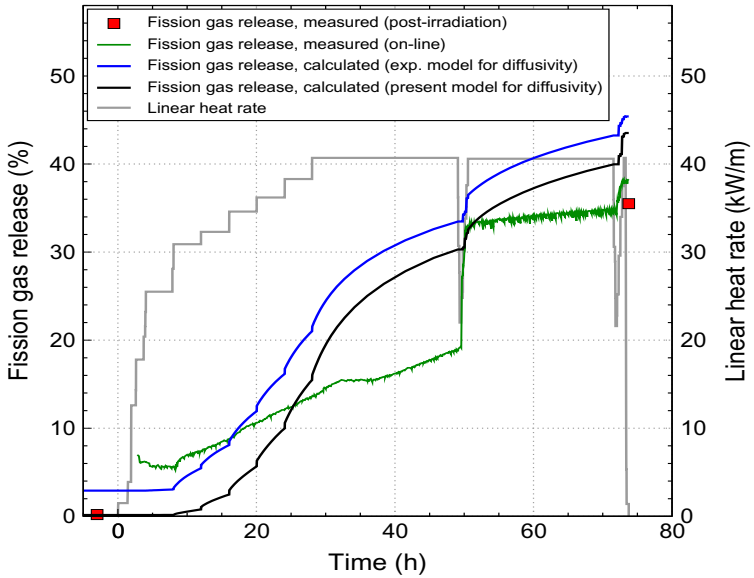
Left: Micrographs of from power pulse tests showing fuel micro-cracking (Top: CABRI REP-Na 5, Lemoine et al., Halifax, 2000. Bottom: NSRR JM-4, Nakamura et al., J. Nucl. Sci. Technol. 33, 1996)

Right: FGR with fuel centerline temperature. The inset shows a shorter time around the power pulse

Atomistic modeling for Xe diffusivity

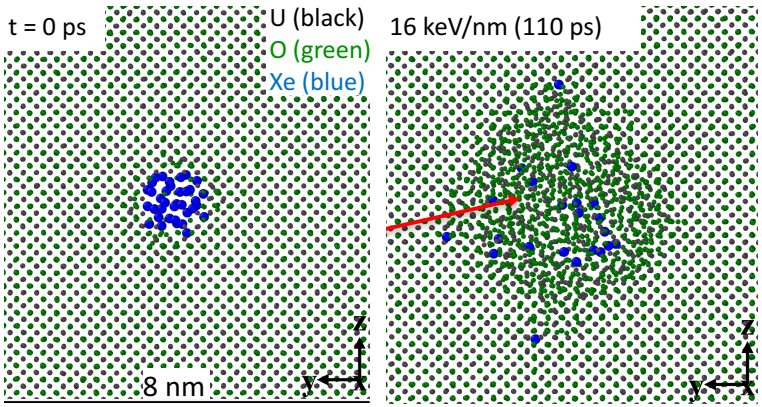
- Atomistic (DFT, empirical potential) modeling for the diffusivity of Xe in the UO_2 matrix is performed at Los Alamos National Lab.
- Early work led to a new diffusivity model that was implemented in BISON (*D.A. Andersson et al., JNM 451, 225, 2014*)
- Further work is in progress at LANL

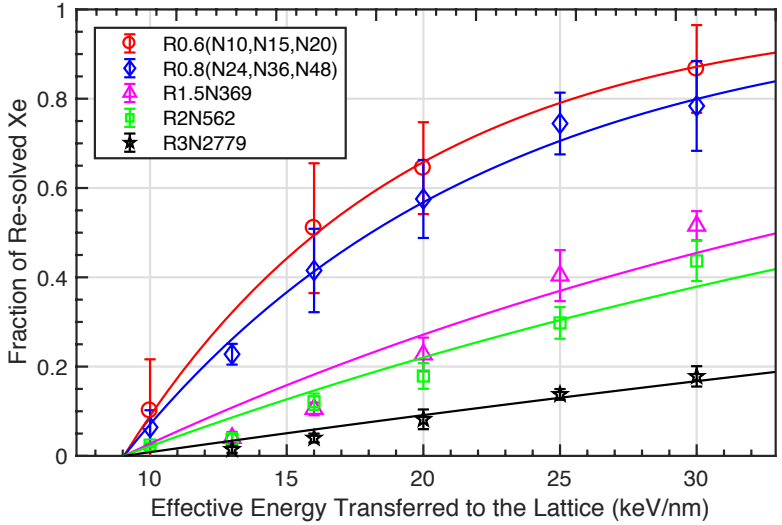


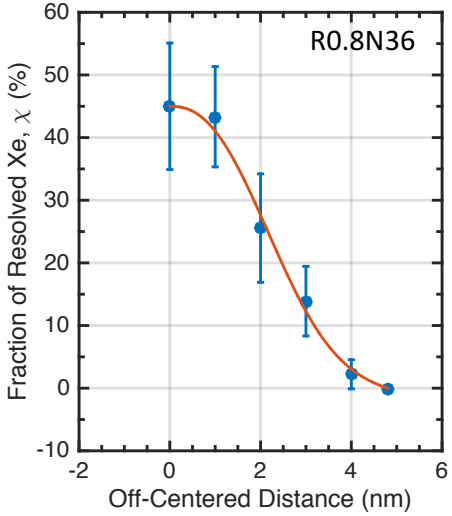


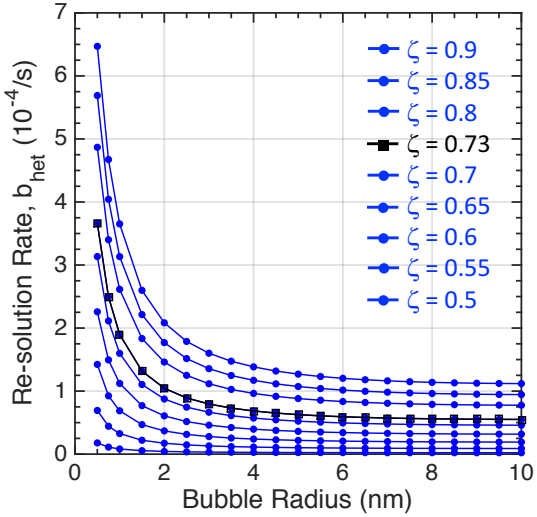
Atomistic modeling for Xe resolution

- Molecular dynamics (MD) calculations for the Xe resolution rate from intra-granular bubbles were performed at Pacific Northwest National Lab. (*W. Setyawan et al., in preparation*)
- Will be used to inform the engineering model in BISON



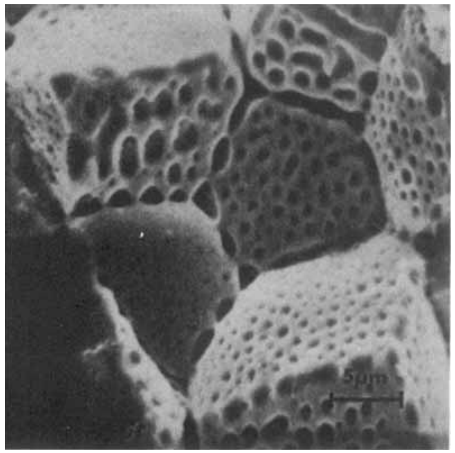




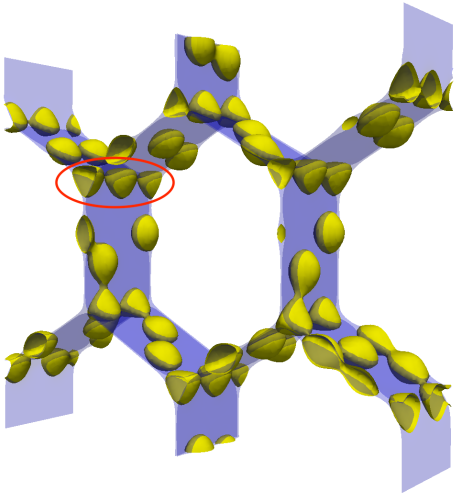


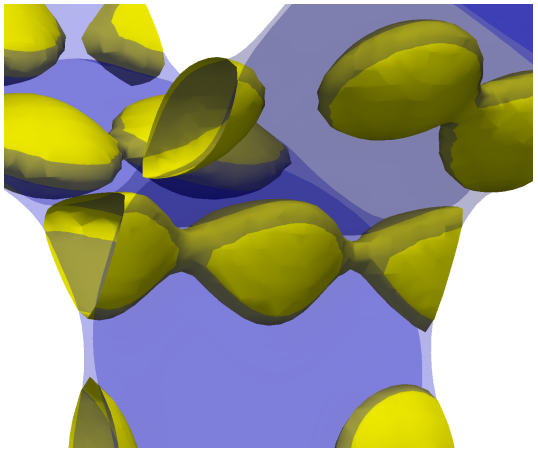
Phase-field modeling for grain-boundary saturation

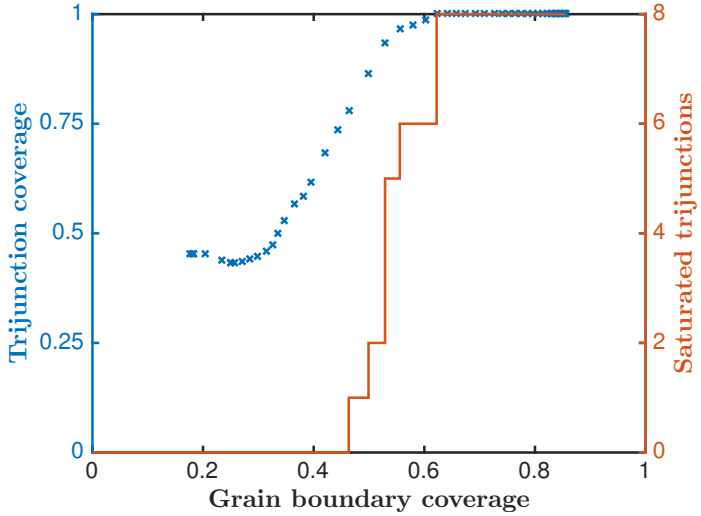
- Phase-field model of bubble evolution at grain faces and edges (triple junctions) was developed at INL
- Grain-edge coverage and saturation was correlated to grain-face coverage
- Can be used to inform the engineering model with thresholds for FGR from the grain edges



Tucker, Radiation Effects, 53, 1980

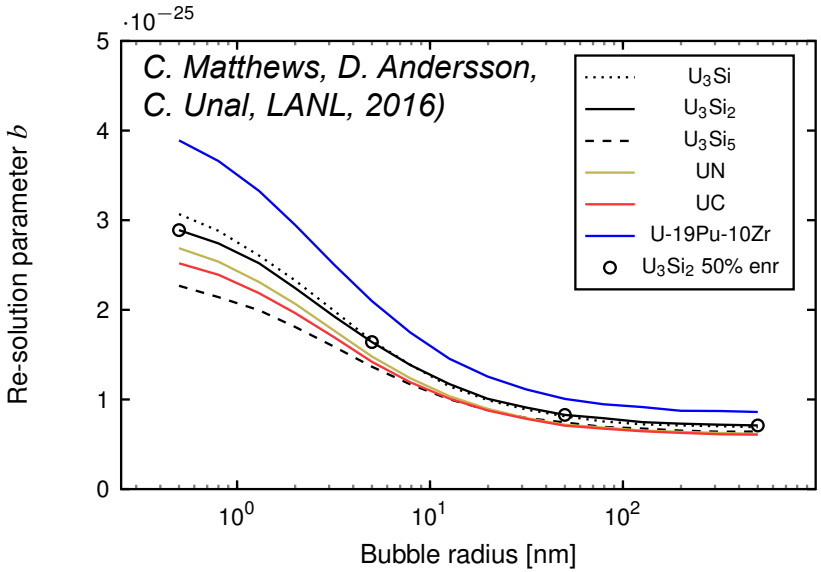


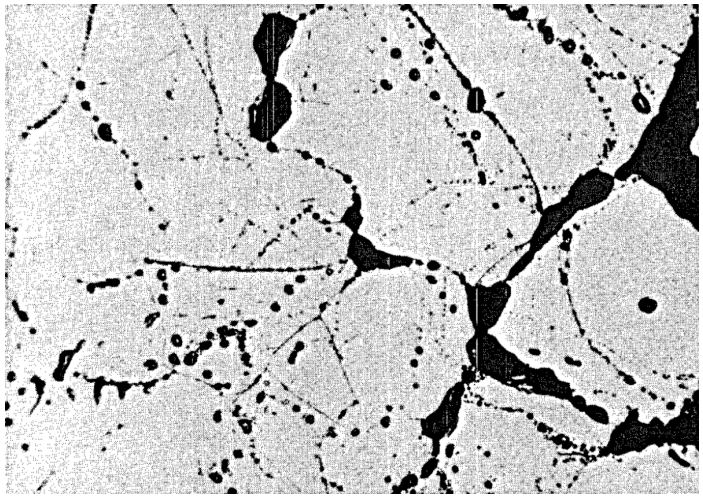




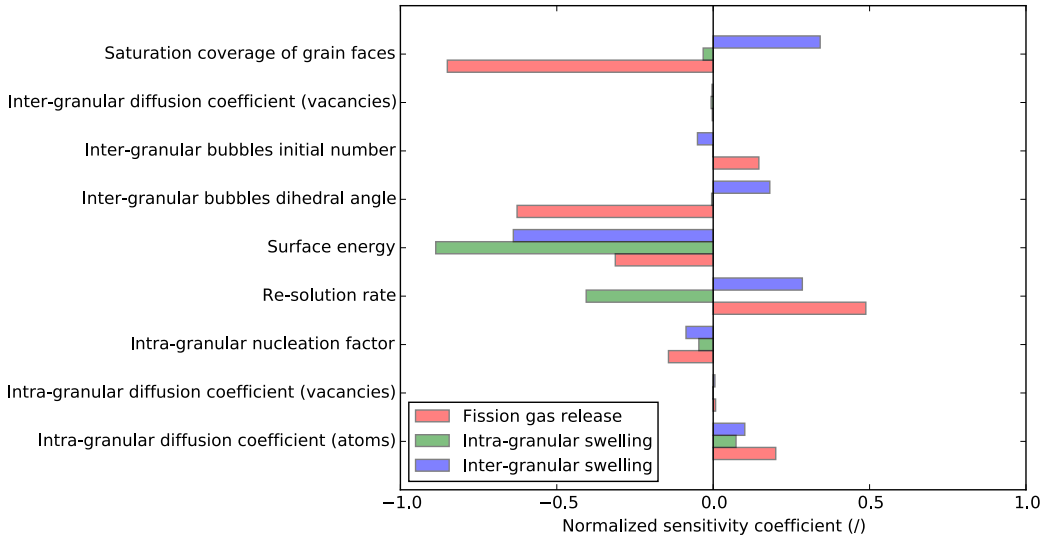
Multiscale fission gas model for U_3Si_2

- Initial model of fission gas behavior in U_3Si_2 for BISON
- Informed by atomistic calculations for the basic parameters (resolution, diffusivity), to fill the experimental data gap
- Sensitivity analysis to help addressing future research



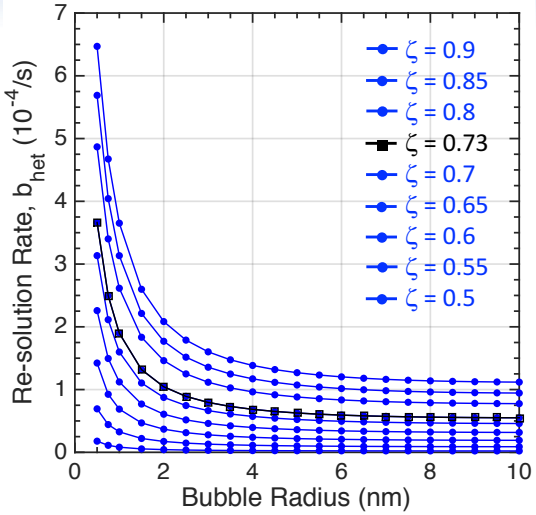


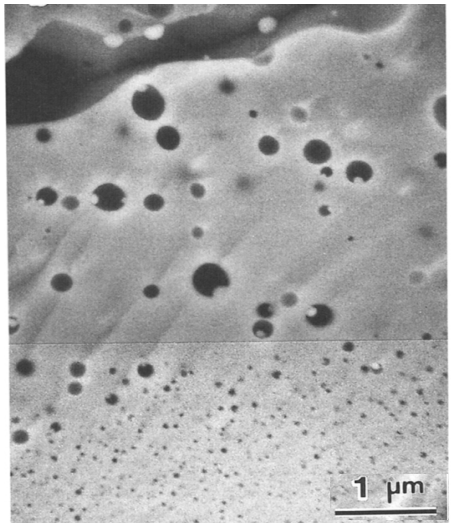
Shimizu, Report NAA-SR-1062, 1965



Outlook

- Inform BISON fission gas models with new parameters from atomistic models of Xe diffusion and resolution
- Extend intra-granular model to bubble coarsening and the associated fuel swelling during transients/ high burnup
- Extend fission gas model to gaseous porosity evolution in the high burnup structure (HBS)
- Continued model validation





Bubble coarsening, Kashibe et al., J. Nucl. Mater. 206, 22, 1993

Acknowledgements

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