Silver Transport in Silicon Carbide From the Atomistic to the Engineering Scale

NSUF Science Review Meeting

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INL

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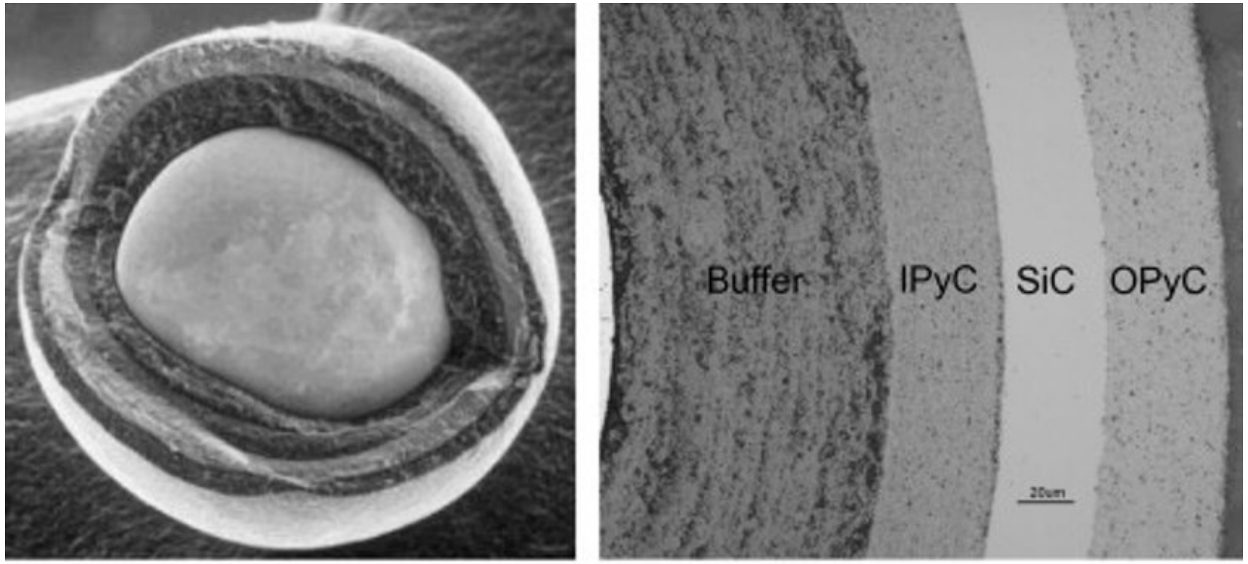
NEAMS
NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Outline

- Background: fission gas release from tri-structural isotropic (TRISO) particles
- A multiscale approach to develop a mechanistic model for silver (Ag) diffusion in silicon carbide (SiC)
- Calculation of the Ag effective diffusivity in SiC
- Application to Ag release from AGR-1 and AGR-2 TRISO particles using BISON
- Ongoing efforts to account for irradiation effects and more microstructure features
- List of publications, reports, presentations, and collaborations resulting from this project

Background: fission gas release from TRISO particles



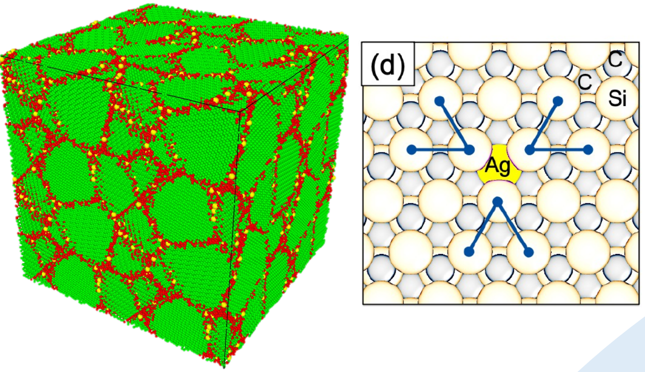
(a) (b)

- The purpose of the SiC layer in TRISO fuel particles is to prevent the escape of fission products produced in the fuel kernel. Ag release is a concern due to the long half-life of the ^{110m}Ag isotope.

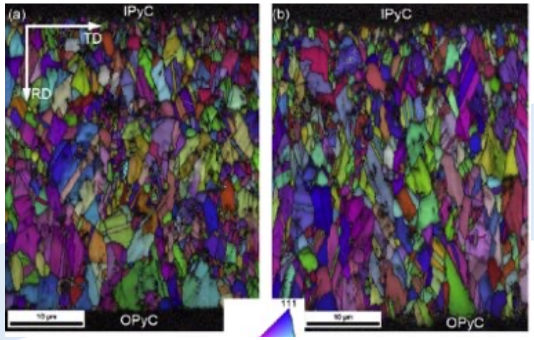
https://www.energy.gov/ne/articles/triso-particles-most-robust-nuclear-fuel-earth
J.D. Hales, et al., Journal of Nuclear Materials, 443.1-3 (2013): 531-543.

A multiscale approach to develop a mechanistic model for Ag diffusion in SiC

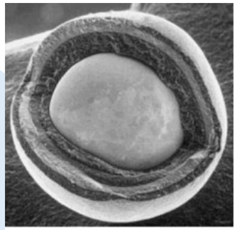
Can we quantify the effect of temperature and SiC microstructure on Ag diffusivity to predict Ag release from TRISO particles?

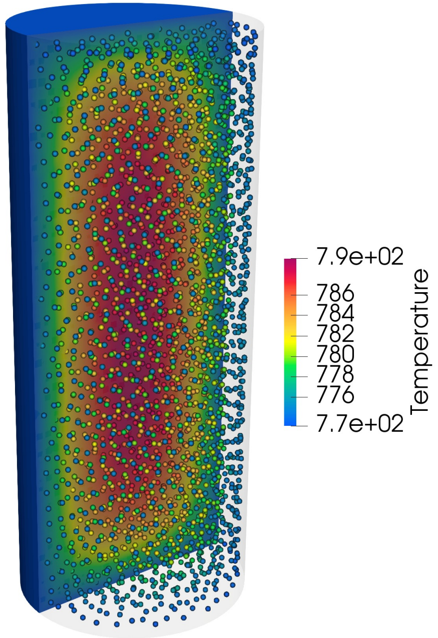


Atomistic calculations of
bulk and grain boundary diffusion



Understand the effect of SiC grain size
and elongation on Ag diffusion with MOOSE

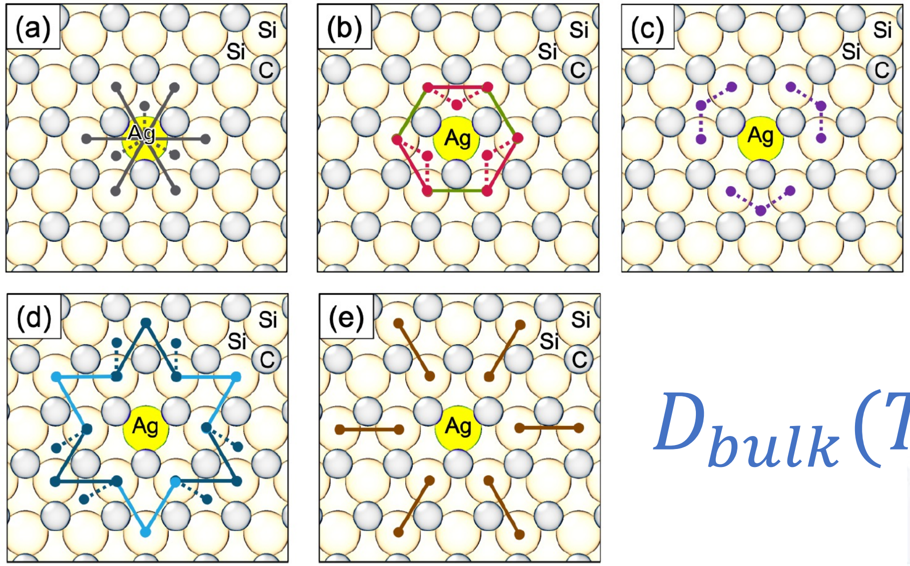




Predict Ag release at the engineering
scale with BISON, and validate against
AGR-1 and AGR-2 measurements

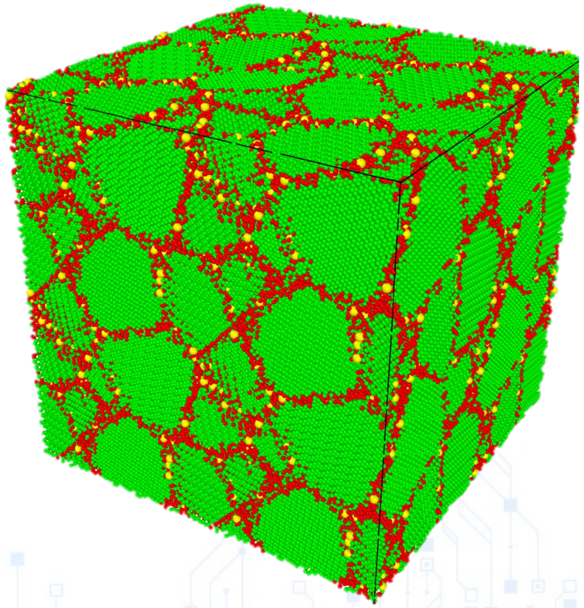
Atomistic calculations of bulk and GB diffusion

- Bulk diffusion in grains is determined using Density Functional Theory (DFT) and kinetic Monte Carlo (kMC) simulations



$D_{bulk}(T)$

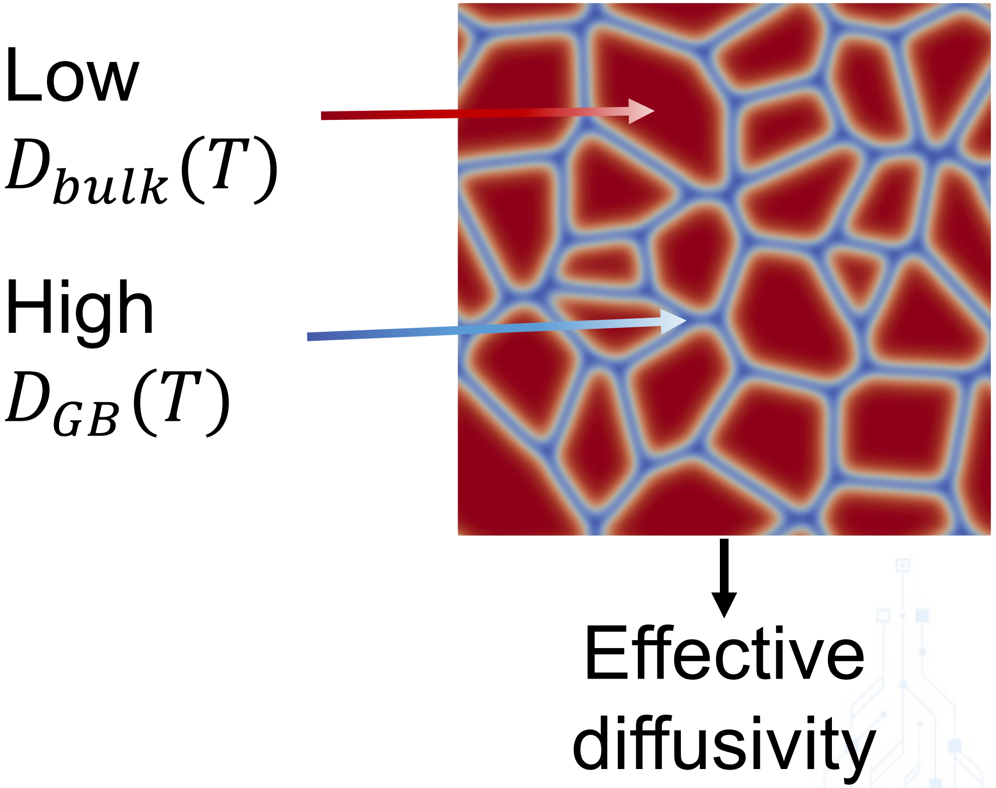
- High-angle grain boundaries (GB) diffusion is determined using molecular dynamics (MD) simulations



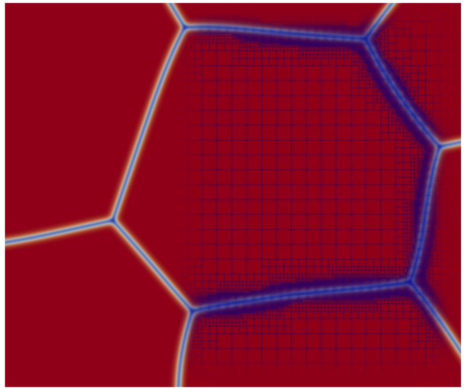
$D_{GB}(T)$

C. Jiang, J.-H. Ke, P.-C. A. Simon, W. Jiang, and L. K. Aagesen. Atomistic and mesoscale simulations to determine effective diffusion coefficient of fission products in sic. Technical Report INL/EXT-21-64633, Idaho National Laboratory, September 2021.

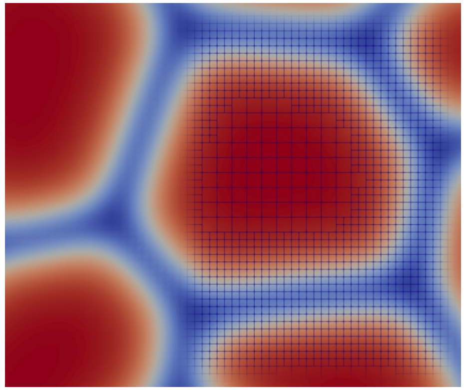
Scaling up to the mesoscale: a challenge



- Using a realistic GB size requires a very fine mesh, which is computationally expensive



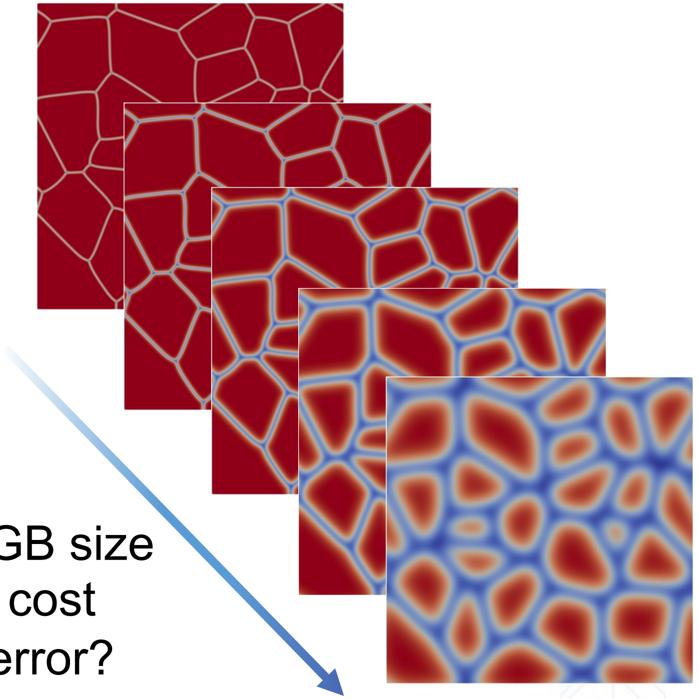
Fine mesh, high cost



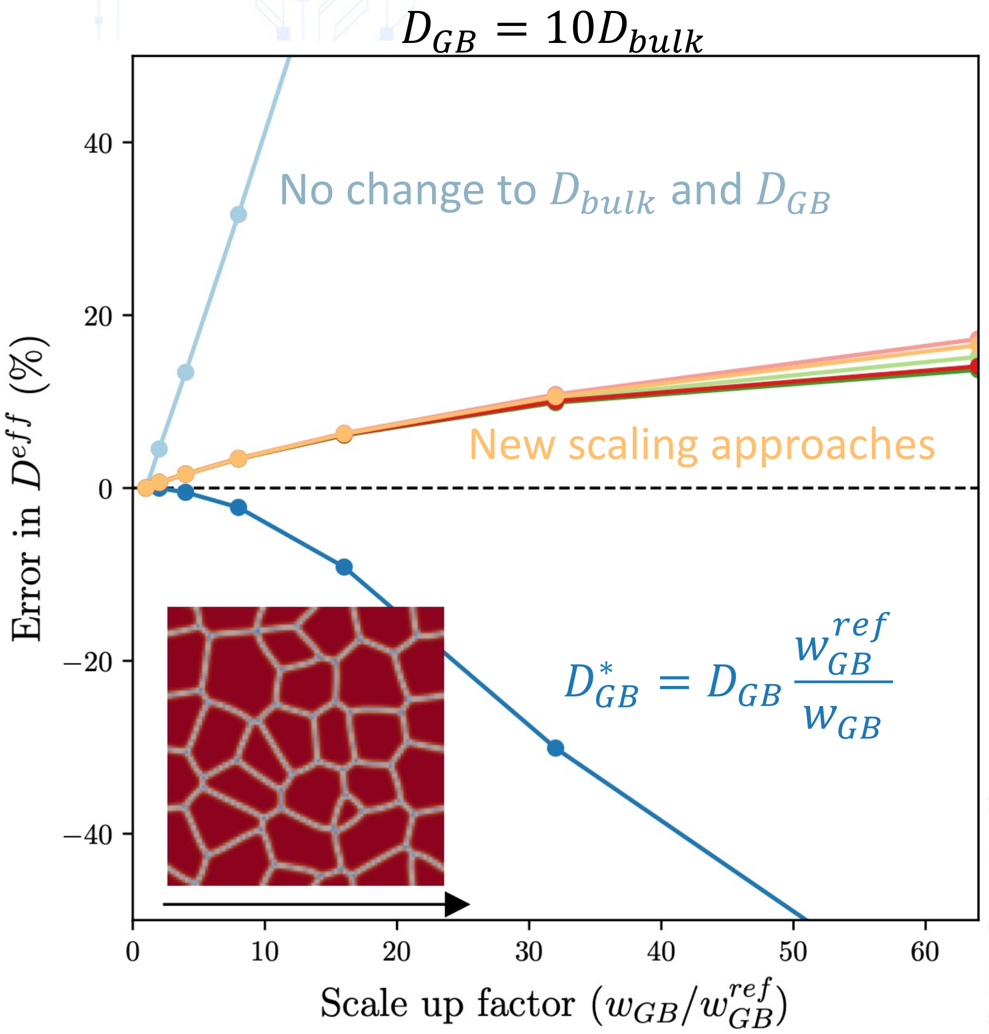
Coarse mesh, low cost

- We need to use artificially large GBs, without introducing errors

Scaling up to the mesoscale while accurately predicting the effective Ag diffusivity

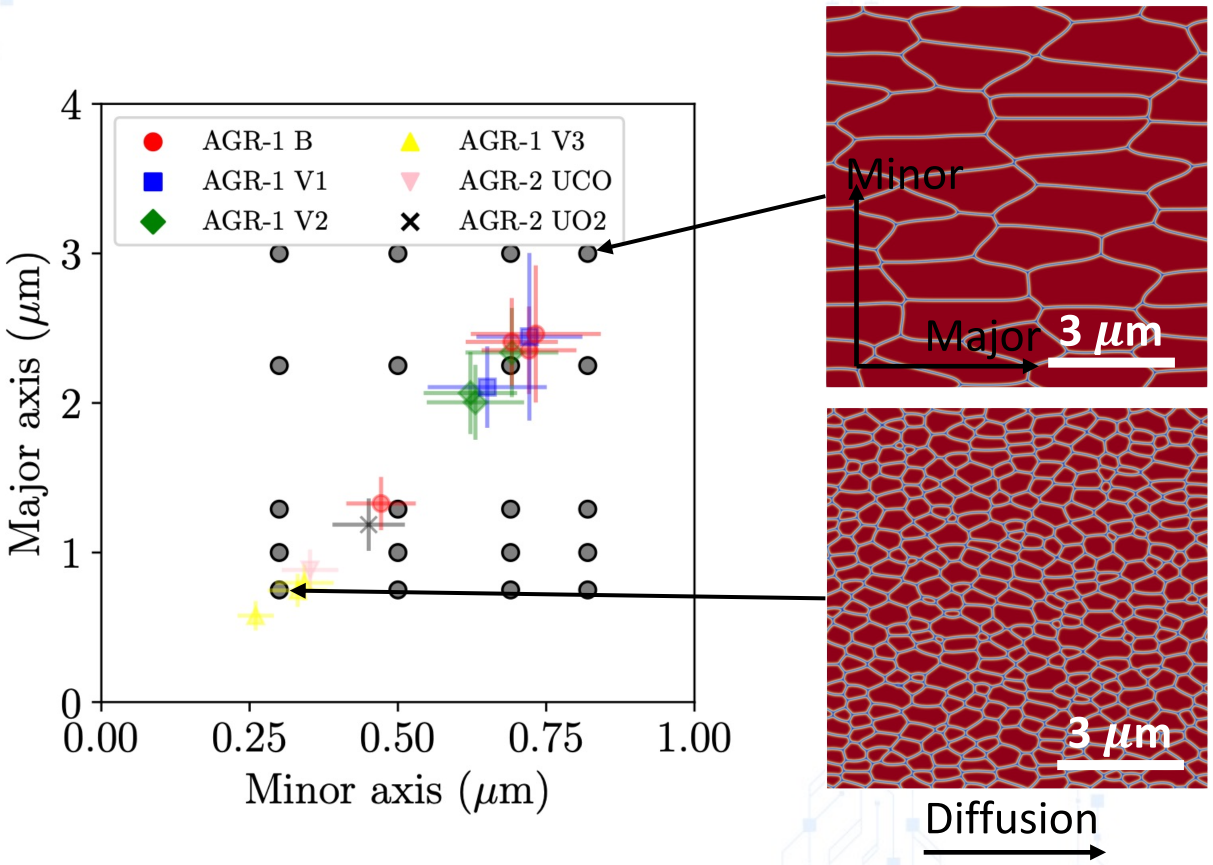


- Increase GB size
- Decrease cost
- Increase error?



A new approach was developed to simulate larger GB sizes without introducing too much error in the final prediction

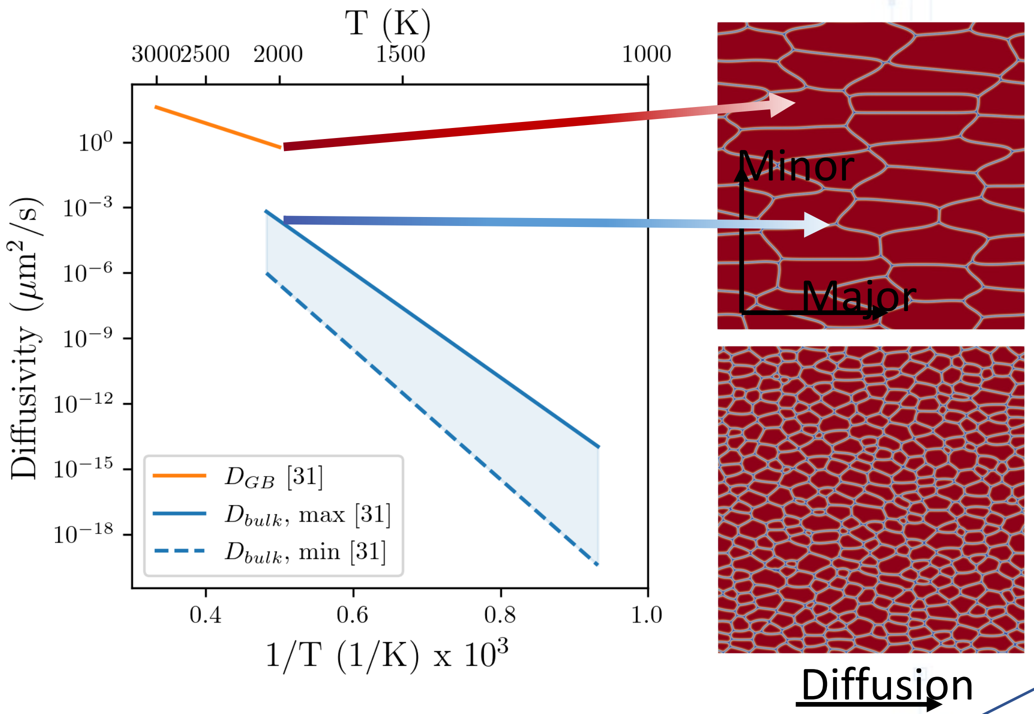
Generating realistic grain structures



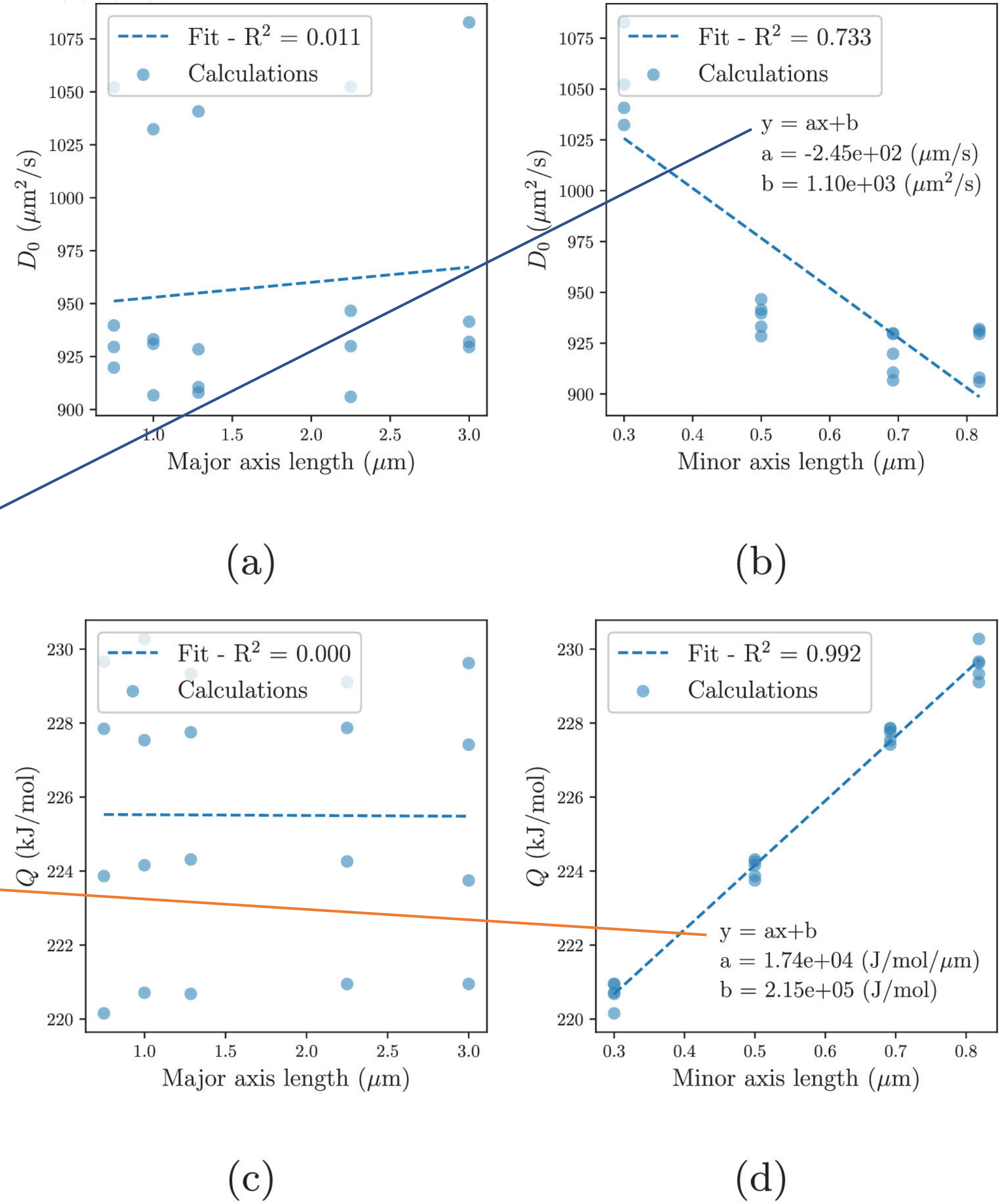
- A higher density of GB is expected to lead to faster diffusion
- Several grain structures with sizes relevant to AGR-1 and AGR-2 materials were generated
- These will be used to quantify microstructure effects on diffusivity

[1] Gerczak et al., J. Nucl. Mater., 480 (2016), pp. 257-270

Calculation of the Ag effective diffusivity in SiC

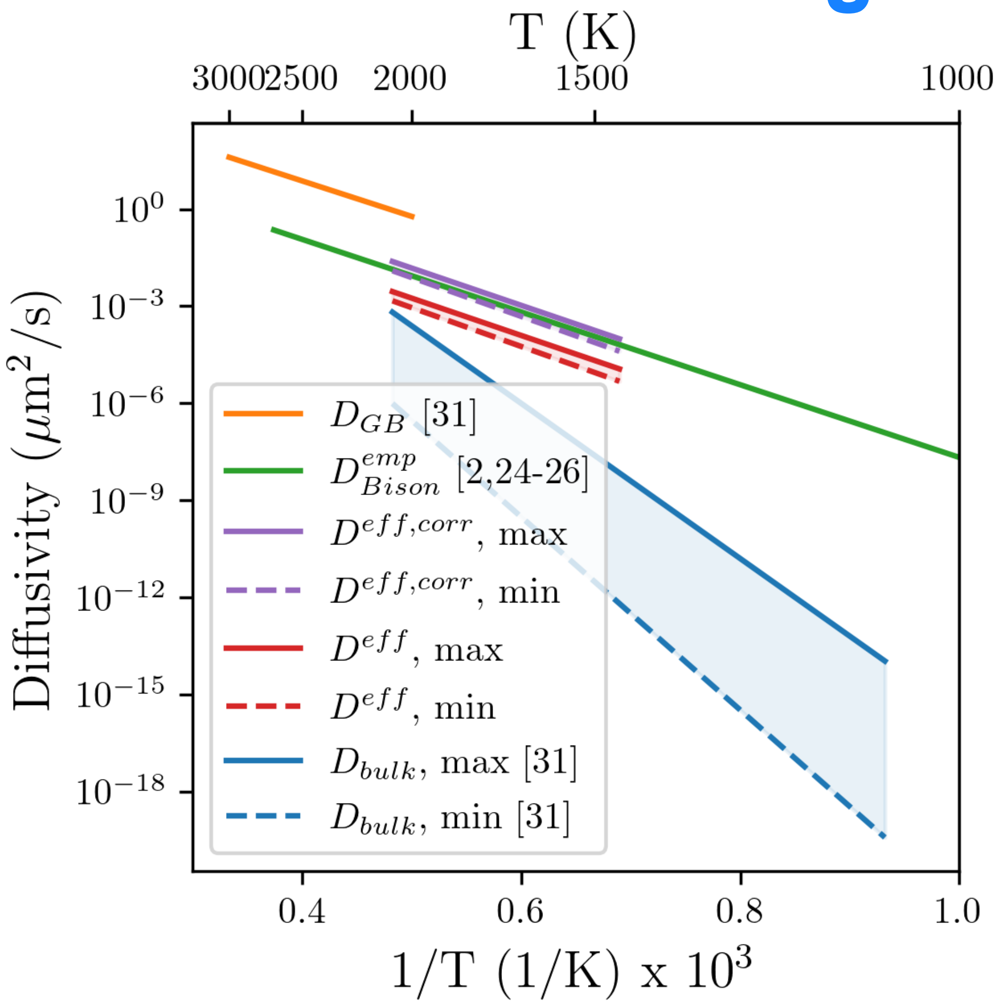


$$D^{eff}(T, m_i) = \left(D_{m,0} + m_i\, D_{m,1}\right) \exp\left(-\frac{Q_{m,0} + m_i\, Q_{m,1}}{RT}\right)$$



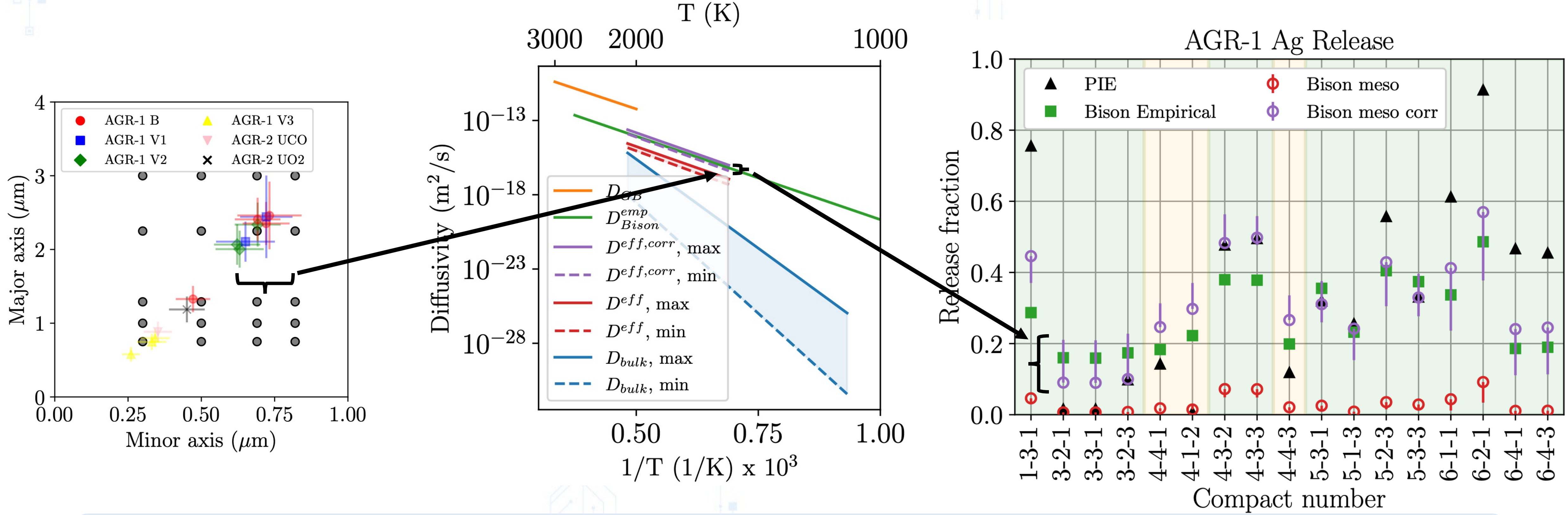
The use of HPC resources was crucial to perform simulations at all the required temperatures and for all the different microstructures

Calculation of the Ag effective diffusivity in SiC



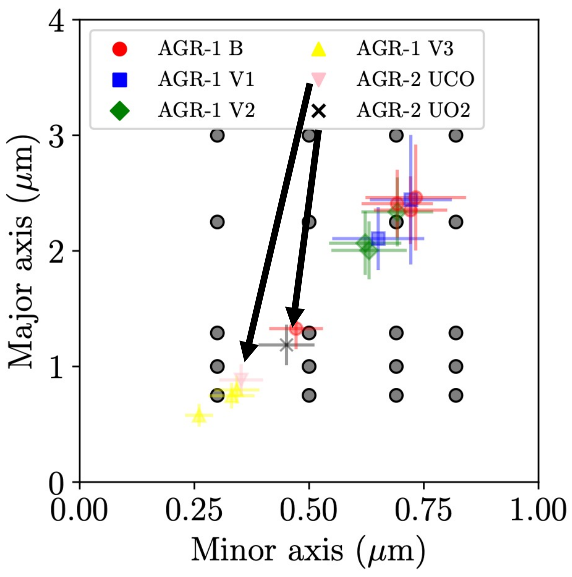
- The multiscale approach accurately predicts the energy barrier of D^{eff}
- Using a corrective multiplier of 8.5 brings D^{eff} to a similar value than the empirical recommended by IAEA
  - Uncertainties
  - Missing physics
- The advantage of the mechanistic approach is that it accounts for microstructure effects

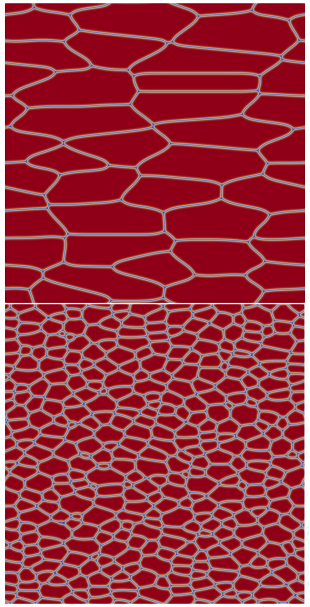
Application to Ag release from AGR-1 using BISON: Quantification of microstructure effects on release

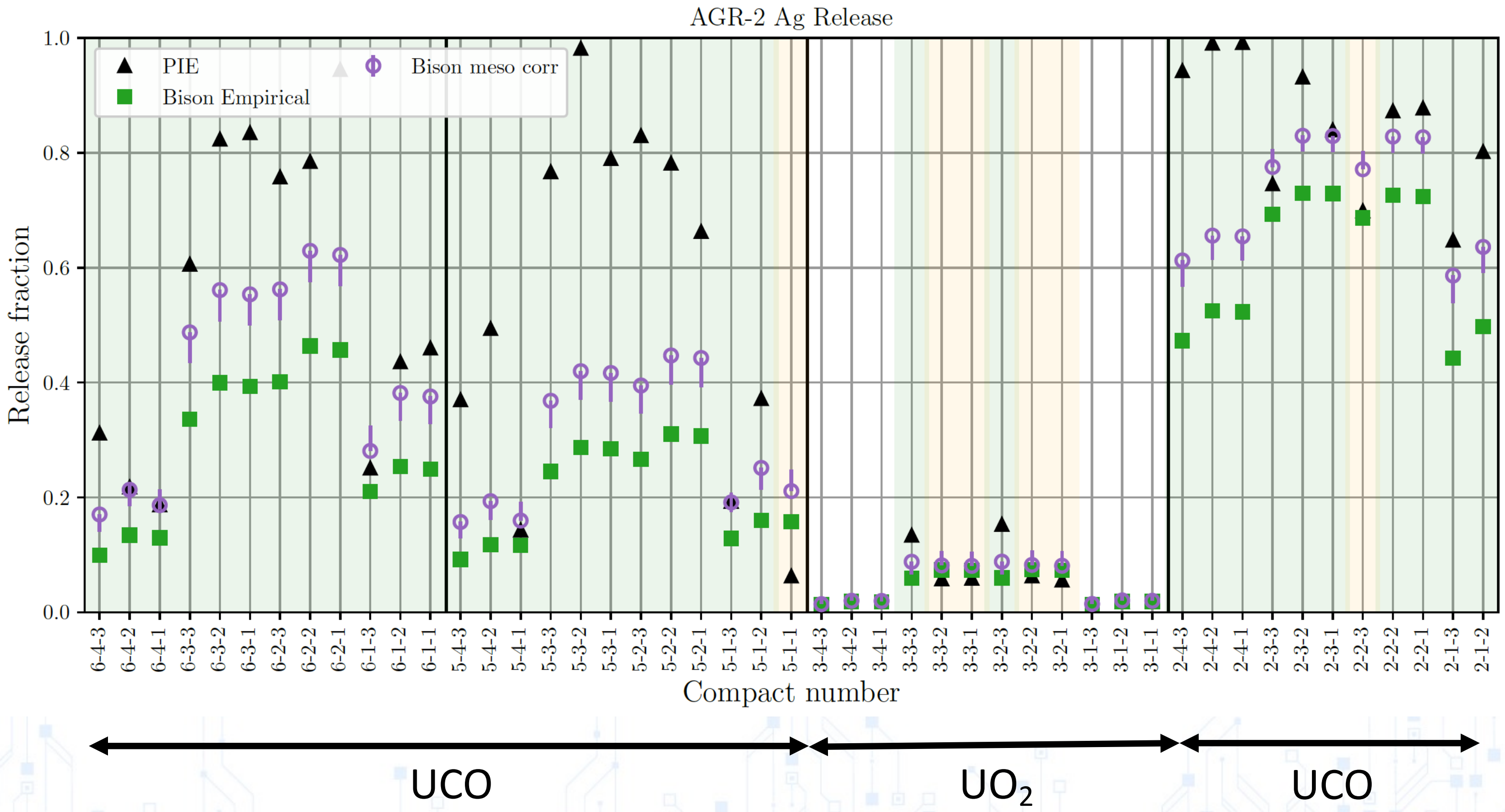


Relatively small variations in grain minor axis size lead to large differences in Ag release fraction. The manufacturing process should promote large grain size along in minor axis.

Application to Ag release from AGR-2 using BISON

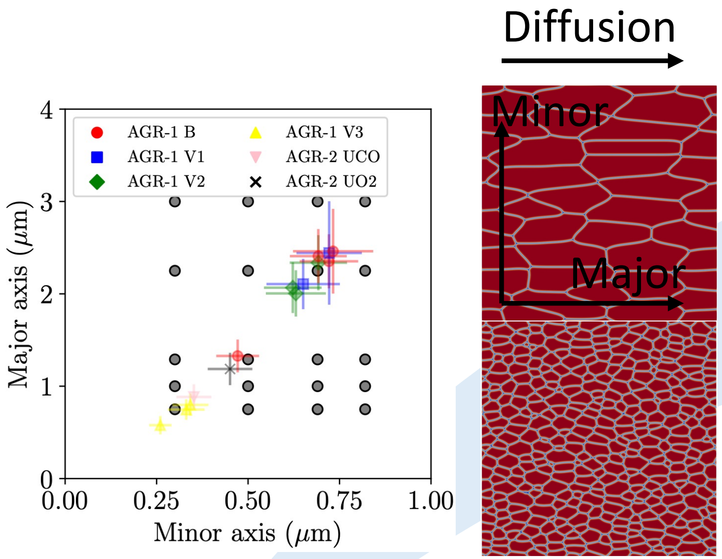




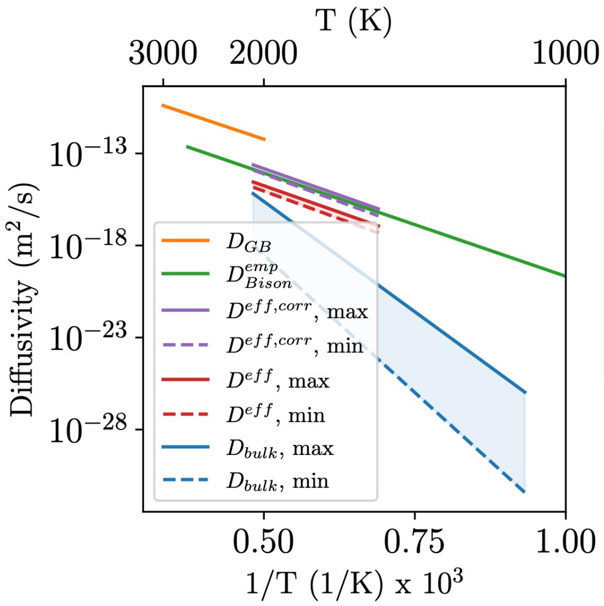


The mechanistic multi-scale approach improves BISON's predictions

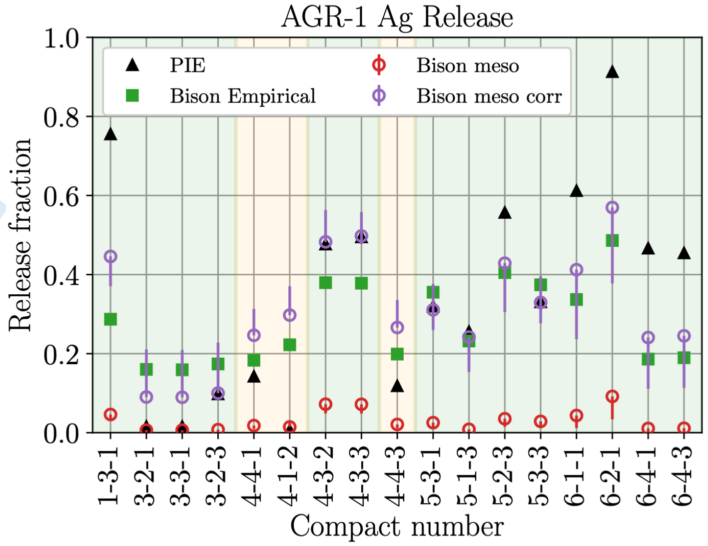
Multiscale calculation of Ag effective diffusivity in SiC



Mesoscale model of Ag diffusion in different polycrystals with different grain sizes



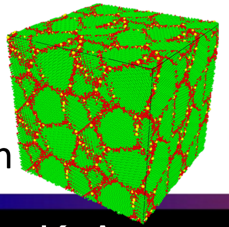
Derivation of a temperature and microstructure-dependent effective Ag diffusivity in SiC



Implementation in BISON and validation against Ag release fraction measurements

We used a mechanistic, multi-scale approach to quantify the impact of SiC grain size on Ag release and improve BISON's predictions.

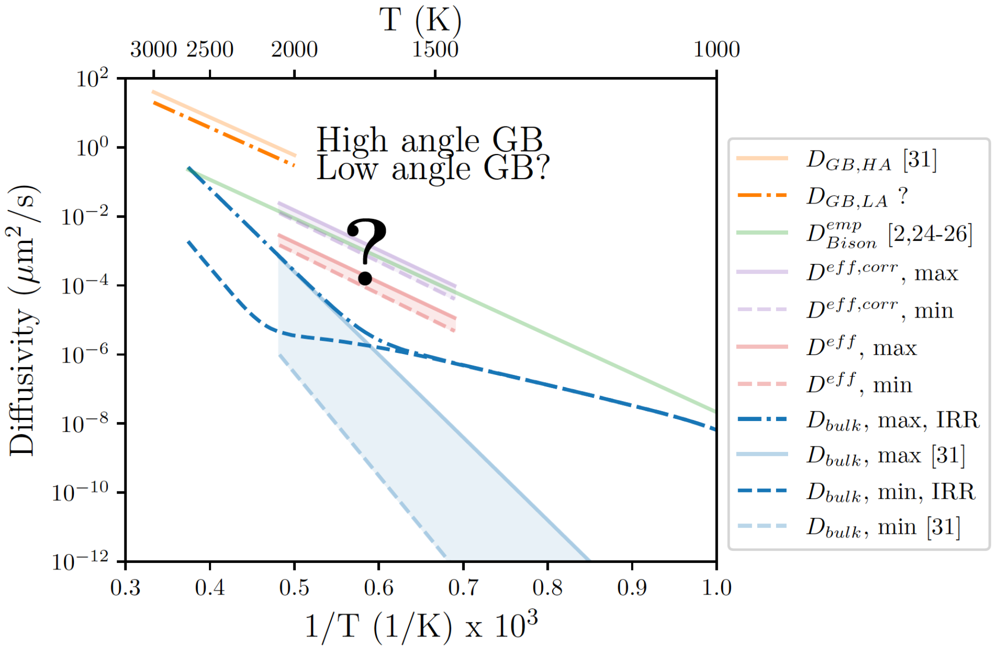
Atomistic calculations of bulk and grain boundary diffusion

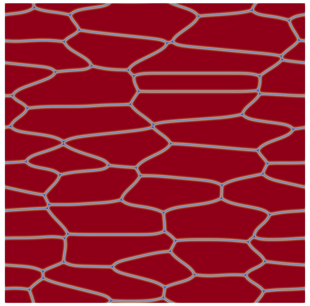


Pierre-Clément A. Simon, Larry K. Aagesen, Chao Jiang, Wen Jiang, Jia-Hong Ke "Mechanistic calculation of the effective silver diffusion coefficient in polycrystalline silicon carbide: application to silver release in AGR-1 TRISO particles ". *Journal of Nuclear Materials*, 563 (2022) 153669

Ongoing efforts

- Include irradiation effects from lower length scale
- Include different diffusivities for different GB types
- Leverage microstructure data (EBSD)





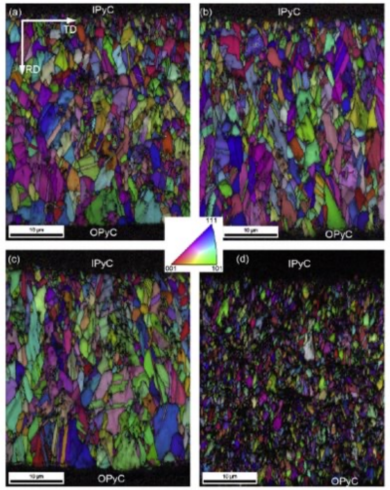


Fig. 2. EBSD generated maps of the SiC layer showing an overlay of the inverse pole figure and image quality map; the reconstructed grain boundaries are shown in black. (a) Baseline, (b) Variant 1, (c) Variant 2, (d) Variant 3. The SiC/IPyC interface is shown at the top of the images. The image quality (IQ) maps generated by EBSD, which is a measure of KBDP quality collected on the scanned area. Un-indexed points, such as the one corresponding to the pyrolytic carbon layers, are shown in black. RD = rolling direction; i.e. grain growth direction of the SiC layer, and TD = transverse direction.

The goal is to develop an effective Ag diffusion coefficient dependent on temperature, grain size, GB types, and irradiation

Products from this project

Journal of Nuclear Materials 563 (2022) 153669

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

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Mechanistic calculation of the effective silver diffusion coefficient in polycrystalline silicon carbide: Application to silver release in AGR-1 TRISO particles

Check for updates

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BISON contribution

INL/EXT-21-64633 Rev. 0

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Atomistic and mesoscale simulations to determine effective diffusion coefficient of fission products in SiC

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Idaho National Laboratory

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Questions?