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Title: Atomic scale simulations for improved CRUD and fuel performance modeling

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Atomic scale simulations for improved CRUD and fuel performance modeling*

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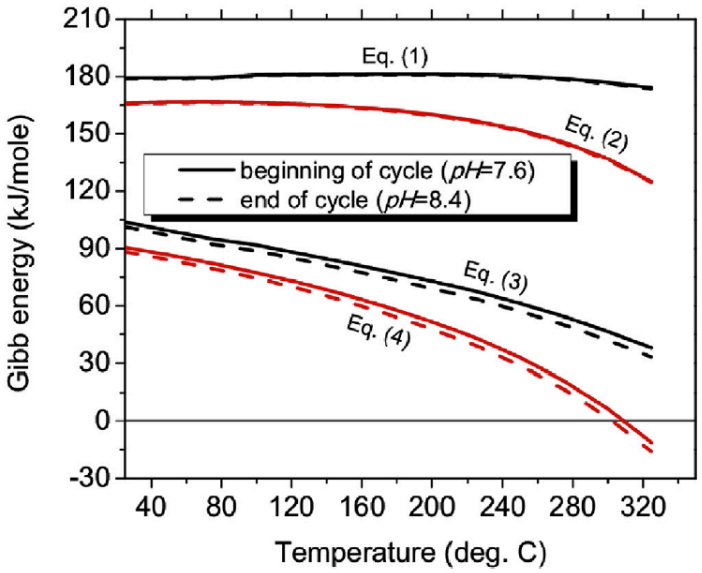
- A more mechanistic description of fuel performance codes can be achieved by deriving models and parameters from atomistic scale simulations rather than fitting models empirically to experimental data. The same argument applies to modeling deposition of corrosion products on fuel rods (CRUD).
- Here are some results from publications in 2016 carried out using the CASL allocation at LANL

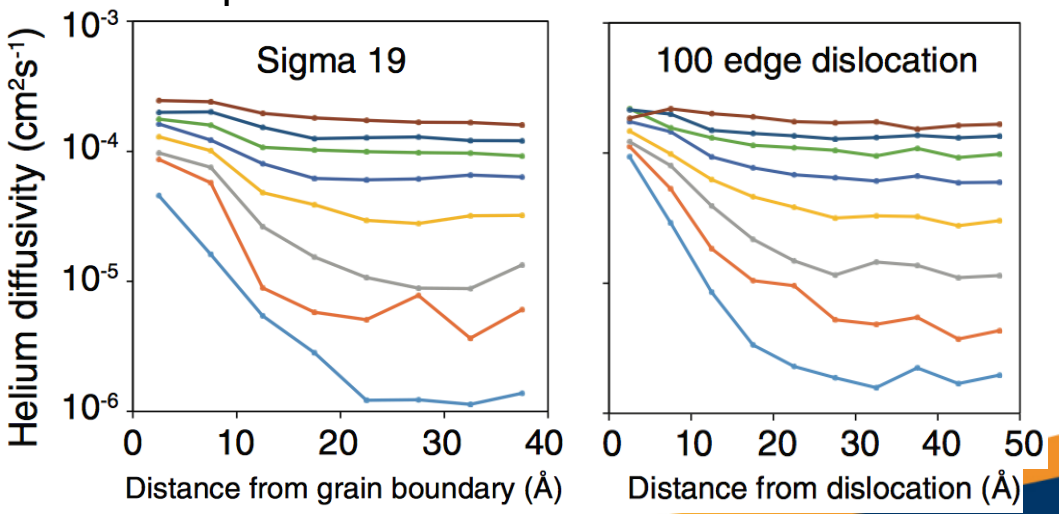
Formation of Ni_2FeBO_5 CRUD

- Combined DFT (VASP) and experimental study to get Gibbs free energy as a function of temperature to inform CRUD deposition in the MAMBA code



Enhanced He diffusion in UO_2 nuclear fuel

- MD simulations (LAMMPS) of dislocation and grain boundary diffusion of He in UO_2
- Enhanced He release mechanism from fuel pellet

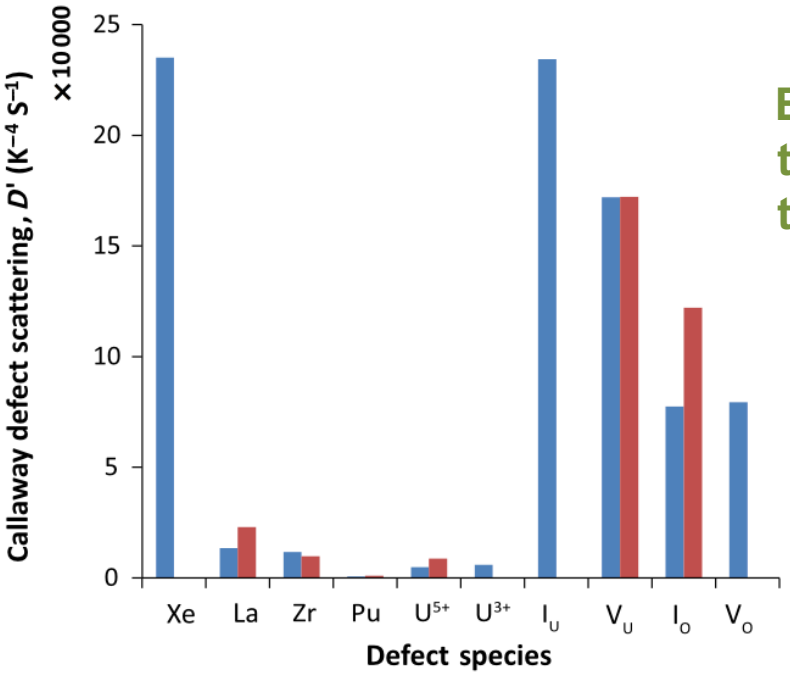


*Work performed using the s11_casl allocation.

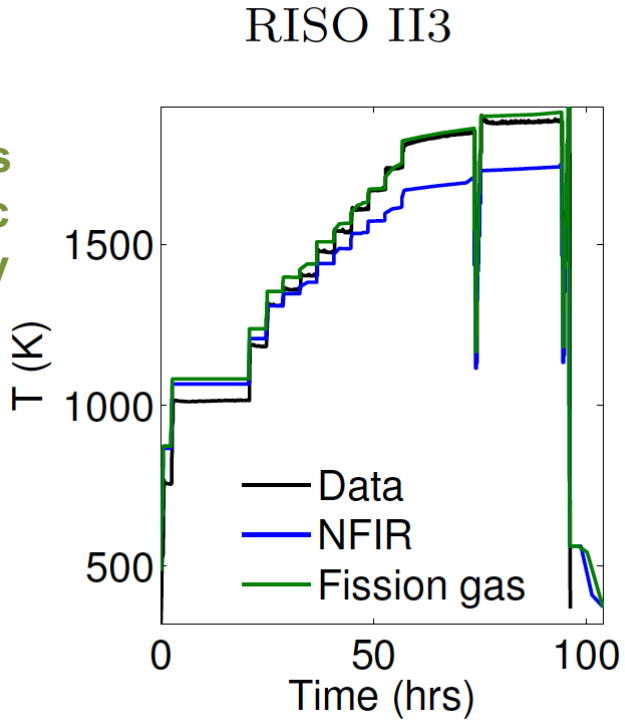
LC for the U.S. Department of Energy's NNSA

Degradation of the thermal conductivity of UO_2 nuclear fuel

- The discrepancy between modeling and experiment is eliminated by using the CRG potential with a method for adjusting MD data (LAMMPS) to account for experimentally determined spin-scattering
- Spin-scattering adjusted MD results are then used to develop scattering parameters for individual defect species for a more mechanistic thermal conductivity model
- Has been successfully implemented by colleagues at INL into the BISON fuel performance code



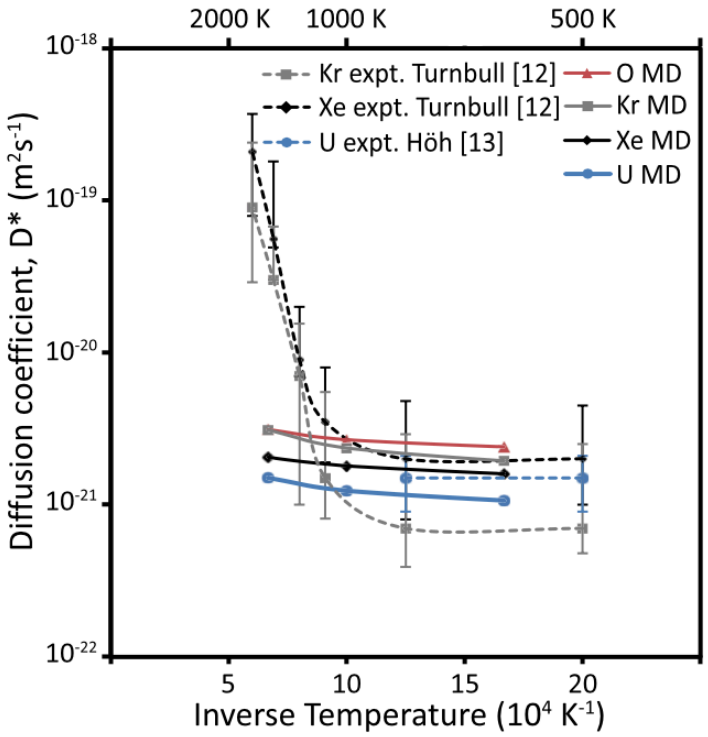
Based on MD results the new mechanistic thermal conductivity in BISON gives improvement



Fission gas diffusion

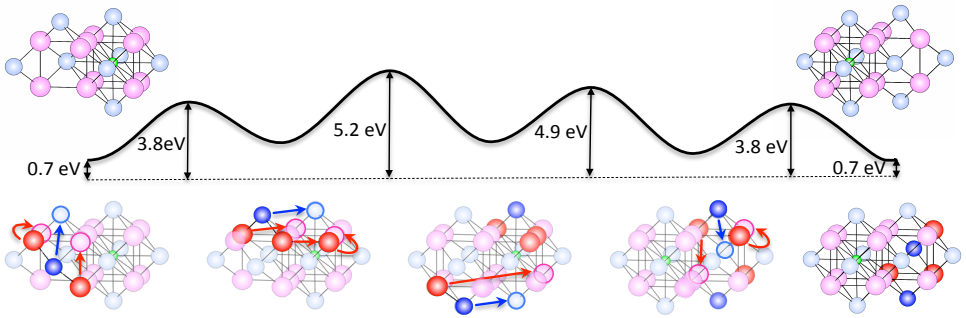
MD simulation (LAMMPS) of radiation driven diffusion (< 1000 K)

- Thermal spikes and cascades in UO_2, ThO_2, and PuO_2 using our new fission gas potential
- Diffusion coefficients can be adjusted according to radiation environment

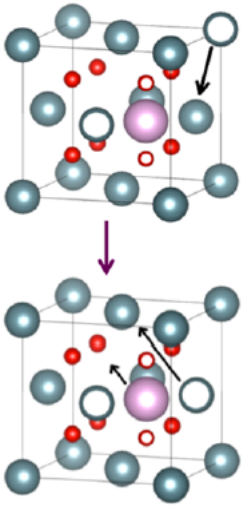


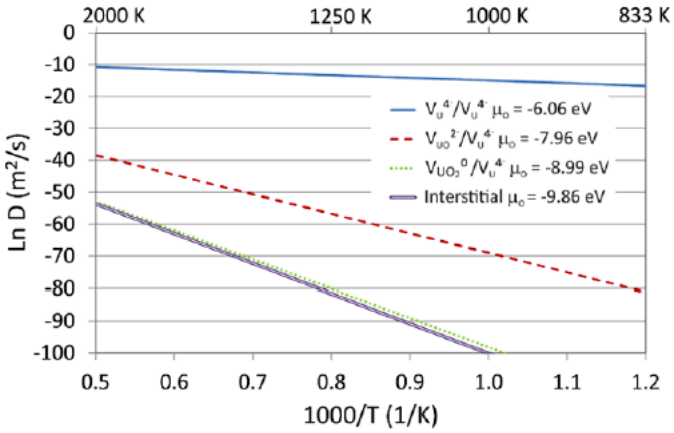
DFT calculations (VASP) for intrinsic diffusion (> 1000 K)

- Investigation of large clusters has highlighted lower Xe diffusion barriers to inform MARMOT



- Combined DFT and empirical potential approach to investigate Kr diffusion coefficients





Publications

1. Zs Rak, CJ O'Brian, D Shin, AD Andersson, CR Stanek and DW Brenner, "Theoretical assessment of bonaccordite formation in pressurized water reactors", *Journal of Nuclear Materials* **474**, 62-64 (2016)
2. E Vathonne, DA Andersson, M Freyss, R Perriot, MWD Cooper, CR Stanek and M Bertolus, "Determination of krypton diffusion coefficient in uranium dioxide using atomic scale calculations", *Inorganic Chemistry*, **10.1021/acs.inorgchem.6b01560** (2016)
3. X-Y Liu, MWD Cooper, KJ McClellan, JC Lashley, DD Byler, BDC Bell, RW Grimes, CR Stanek and DA Andersson, "Molecular dynamics simulation of thermal transport in UO_2 with intrinsic defects and fission products", *Physical Review Applied* **6**, 044015-044033 (2016)
4. MWD Cooper, CR Stanek, JA Turnbull, BP Uberuaga and DA Andersson, "Simulation of radiation driven gas diffusion and self-diffusion in UO_2 at low temperature", *Journal of Nuclear Materials* **481**, 125-133 (2016)
5. MWD Cooper, N Kuganathan, PA Burr, MJD Rushton, RW Grimes, CR Stanek and DA Andersson, "Development of Xe and Kr empirical potentials for CeO_2, ThO_2, UO_2 and PuO_2", *Journal of Physics: Condensed Matter* **28**, 405401-405408 (2016)
6. COT Galvin, MWD Cooper, PCM Fossati, CR Stanek, RW Grimes and DA Andersson, "Pipe and grain boundary diffusion of He in UO_2", *J. Phys.: Condens. Matter* **28**, 405002-4050012 (2016)
7. MWD Cooper, CR Stanek, X-Y Liu and DA Andersson, "A comment on the thermal conductivity of $(U,Pu)O_2$ and $(U,Th)O_2$ by molecular dynamics with adjustment for phonon-spin scattering", *MRS Advances* **1**, 2483-2487 (2016)
8. M. R. Tonks, X.-Y. Liu, D. Andersson, D. Perez, A. Chernatynskiy, G. Pastore, C. R. Stanek and R. Williamson, "Development of a multiscale thermal conductivity model for fission gas in UO_2", J. Nucl. Mater. **416**, 89 (2016)

Talks

- 1 invited talk at TMS 2016 and 1 invited talk at ANS 2016
- 3 talks at MRS Spring 2016 and 3 talks at NuMat 2016