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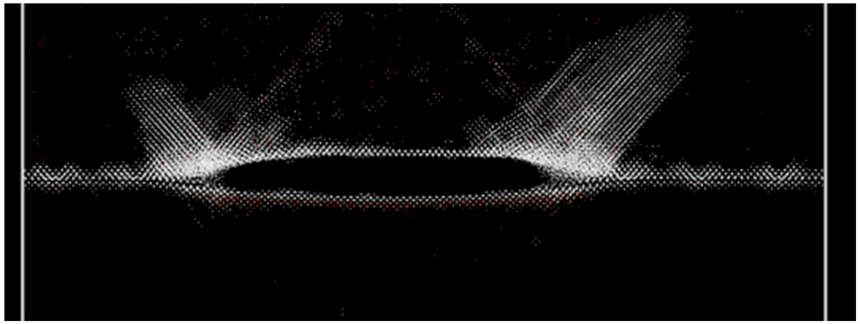
Sandia National Laboratories

Delamination of U/Zr interfaces: an atomistic study



Elton Chen
Georgia Institute of Technology

Supervised by
Rémi Dingreville
Org. 6233

6220/6230 summer student mini-symposium
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U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration
LDRD Laboratory Directed Research & Development

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Outline

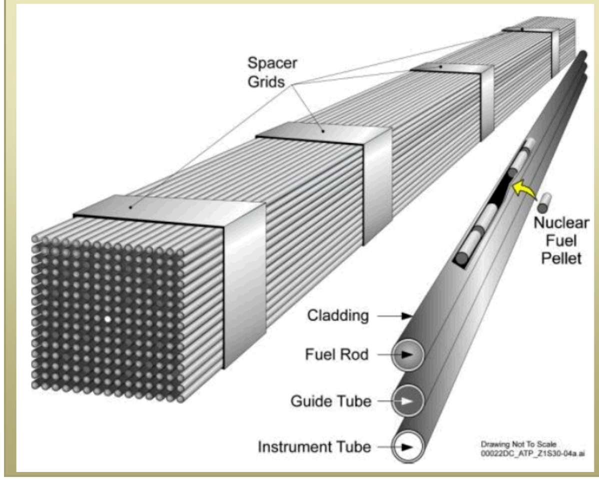
1. Characterization of pellet/clad debonding

2. Why use atomistic modeling

3. Modeling complex U/Zr interfacial structure under harsh environments

4. Conclusion

What is pellet-clad debonding



High temperature
+
Irradiation environment
+
Fission products
+
Swelling

Interfacial inter-mixing: Adsorption, diffusion and reaction

Transport through oxide or access at stressed/weakened defects sites

Crack initiation

Crack growth and propagation

- A crack may be trapped and grow between the pellet and the clad under mixed-mode.
- Effects affecting interfacial debonding:
  - **Interface microstructure/chemistry:** interfacial defects, segregation, intermixing.
  - **Environment:** subcritical debonding, irradiation-induced defects.

Why use atomistic modeling

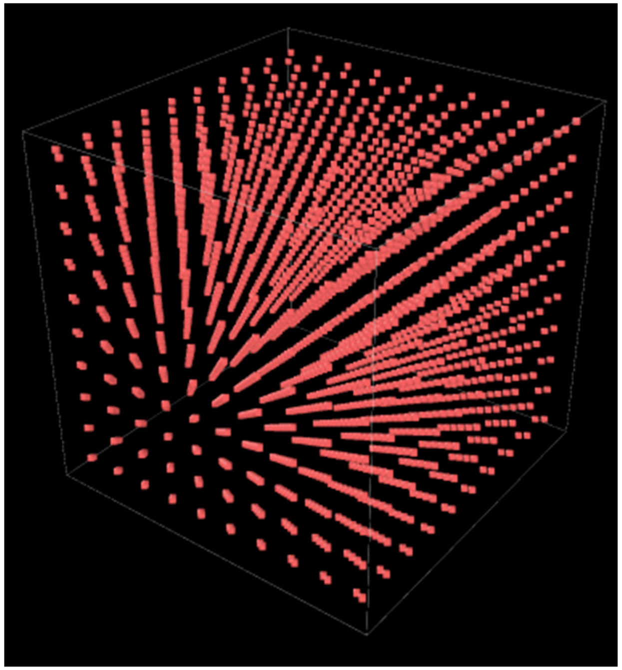
- **(Experimental) characterization of pellet/clad interfaces are difficult and costly:**
  - A lot of the phenomena (radiation, intermixing) take place at the atomic scale
  - Experiments are difficult (hazardous mat'l…)

- **What atomistic simulations can bring:**
  - Data production (thermo, structure) ➢ mesoscopic codes
  - Identification, comprehension and characterization of microscopic mechanisms
  - Interpretation of experimental results

Nuts and bolts of molecular dynamics

$$F_i = m \cdot a$$
$$v_f = v_i + a \cdot t$$
$$d = v_i \cdot t + 0.5\left(a \cdot t^2\right)$$

Newton's 2nd Law & Kinematic Equations



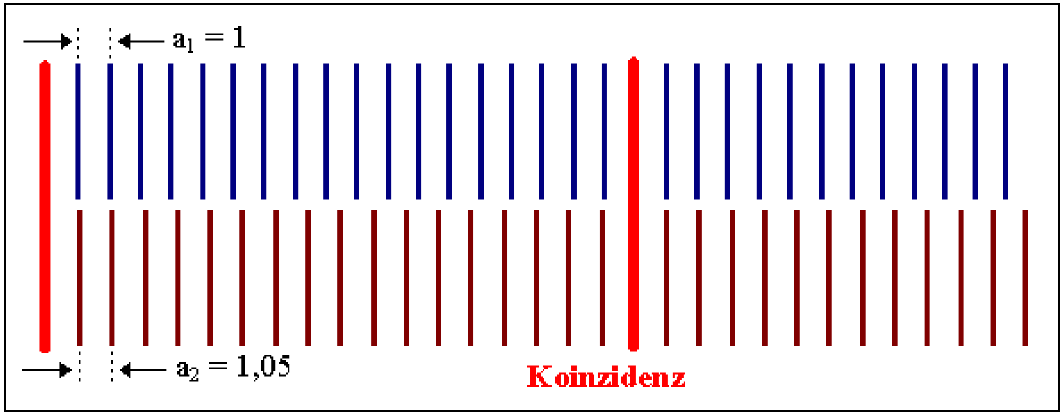
10 x 10 x 10 Bulk BCC Lattice

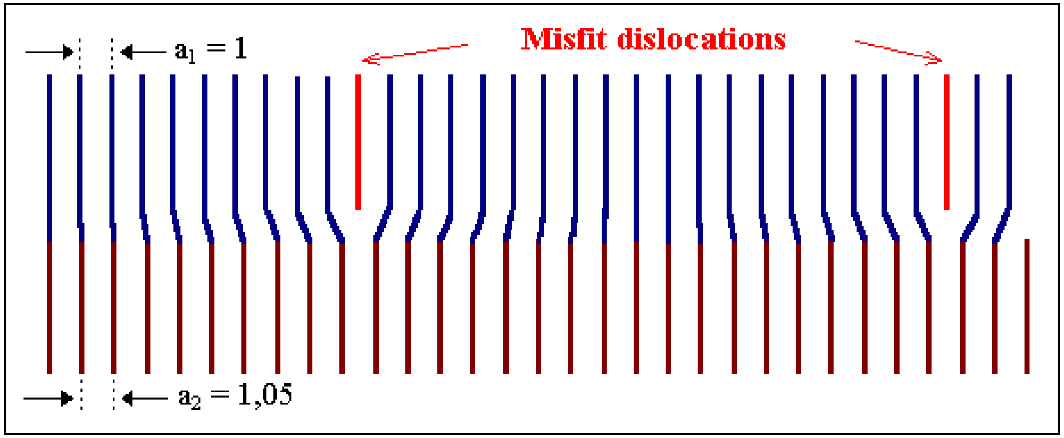
- **Basics:**
  - Integration of motion equations with interaction between atoms via empirical potentials
  - System size ranging from 10^5-10^7 at. (extended defects)
  - **Limitations:** No description of electron and time limited to few ns.

Modeling complex U/Zr interfaces and their behavior in harsh environments

- **Getting the right interface structure**
  - Calculate structural misfit of interfaces
  - Construct misfit interfaces with different orientation
  - Analyze & compare to theory for interfacial defects content
- **Modeling the interfacial radiation-induced intermixing**
  - Introduce interfacial intermixing by sequential PKA cascade
  - Monte Carlo consecutive cascade
- **Modeling the interface delamination**
  - Calculate crack yield condition
  - Crack Insertion into interfacial system
  - Record decohesion behavior

Misfit interface:
Accommodation by interfacial defects

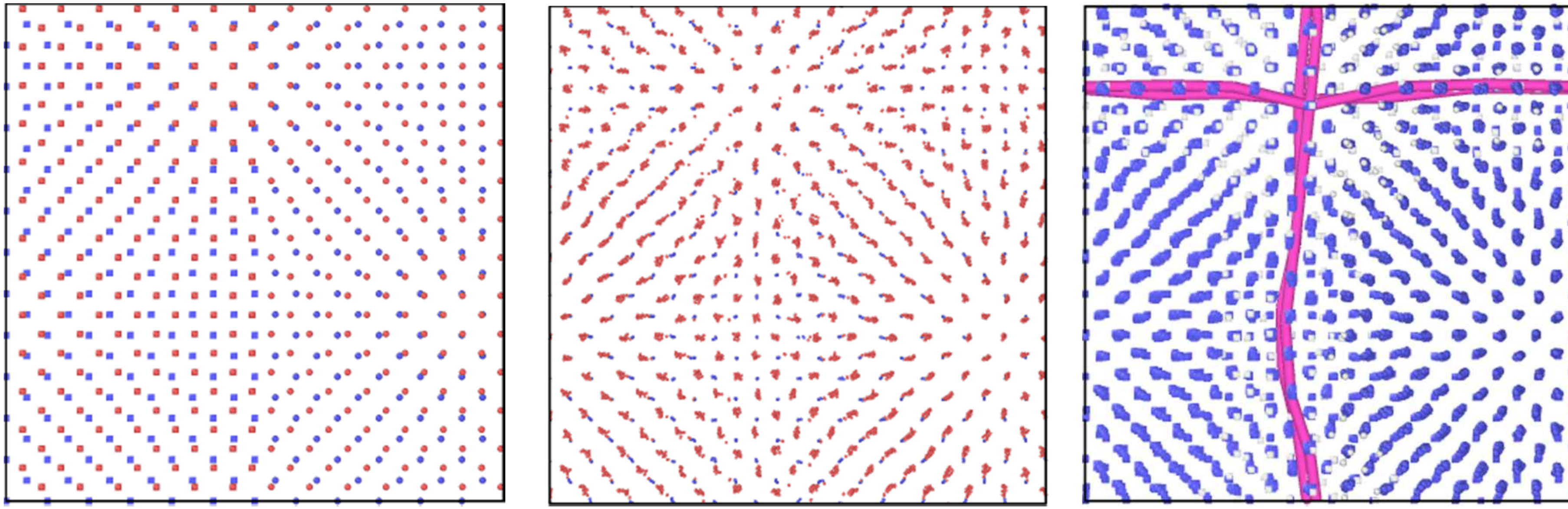




Definition of interfacial misfit: $$f = 2\frac{n \cdot a_1 - m \cdot a_2}{n \cdot a_1 + m \cdot a_2}$$

Misfit dislocation network

Initial Configuration | Post Minimization | Defect analysis

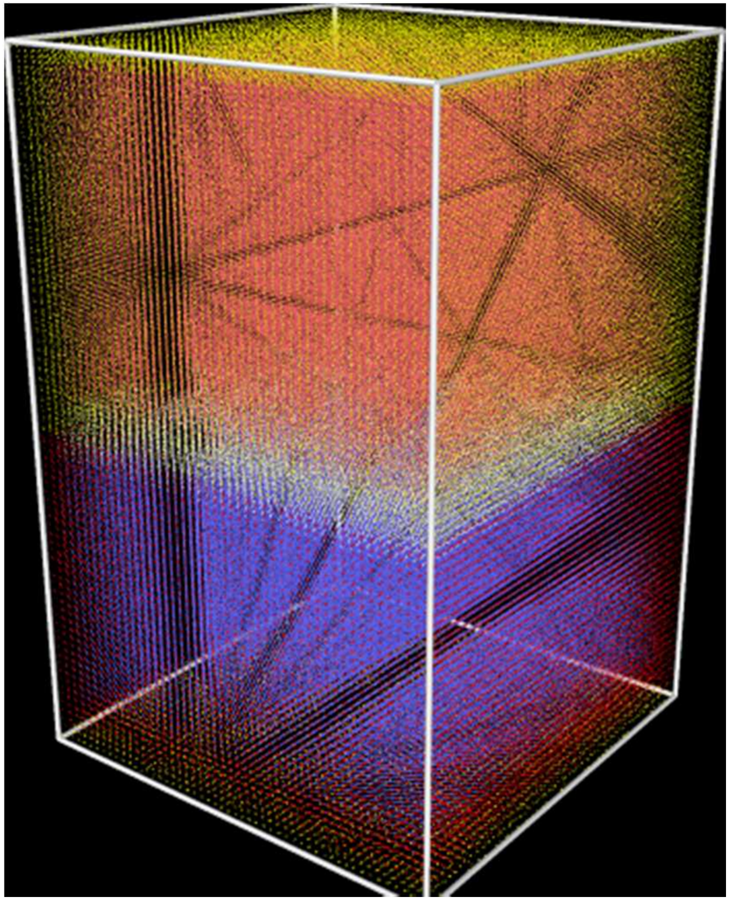


Red – U Lattice
Blue – Zr Lattice

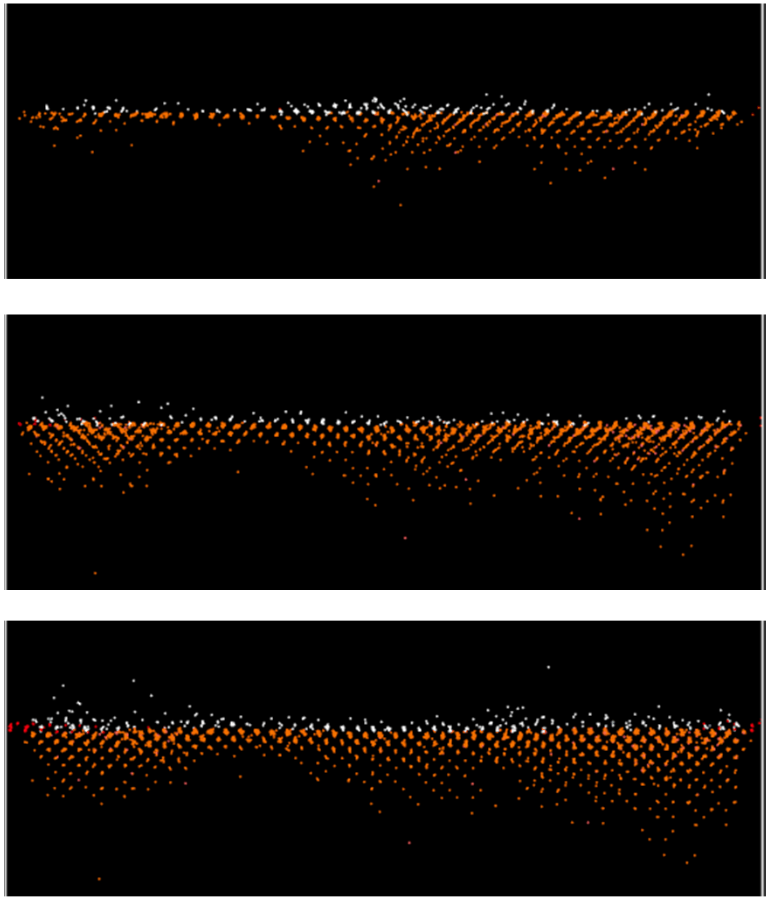
- Defect structure correlates with theoretical comparison

Revisiting the Al/Al2O3 Interface: Coherent Interfaces and Misfit Accommodation, G. Pilania, B. Thijsse, R. Hoagland, I. Lazic, S. Valone & X. Liu. *Scientific Reports* **4**, Article number: 4485 (2014)

Radiation-induced intermixing



Yellow/Red – Temperature Boundary
White – Interfacial Boundary
Pink – Bulk U Lattice
Blue – Bulk Zr Lattice



Orange – U Atoms intrusion in Zr Lattice
White – Zr Atoms intrusion in U Lattice

- As expected, U has greater penetration depth

Interfacial delamination: procedure

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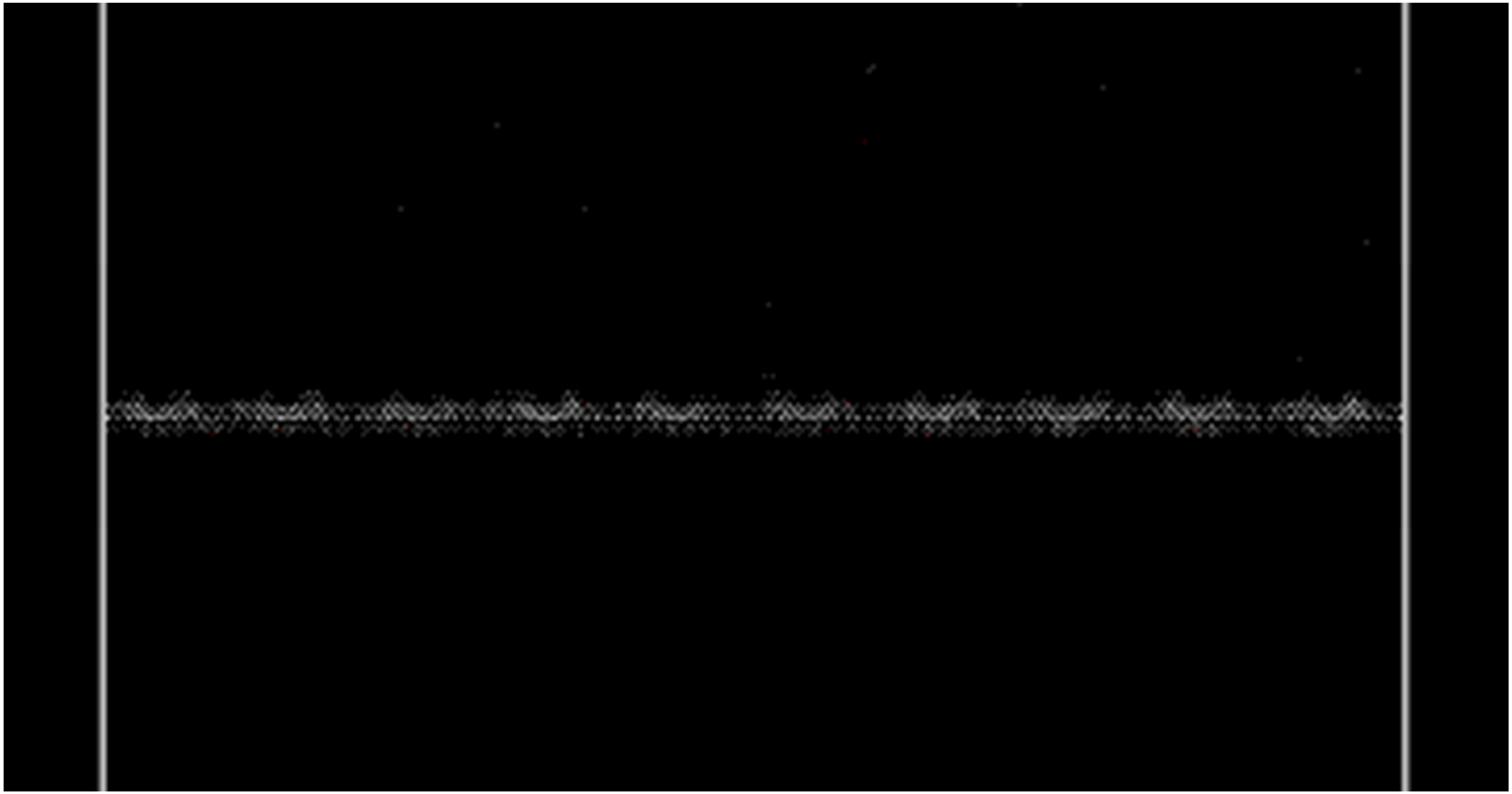
- **Step 1** Build Interface Structure
- **Step 2** Minimize System at 0K
- **Step 3** Equilibrate in NPT ensemble
- *** Step 4** Introduce Radiation Damage
- **Step 5** Preload Tension in NPT ensemble
- **Step 6a** Introduce Crack by Screening
- **Step 6b** Relax in NVT ensemble

- Griffith yield criterion: $\sigma_f \sqrt{a} = \sqrt{\frac{EG}{\pi}}$

Stunt computing: crack propagation



-5GPa pressure loading | 30ps relaxation | Adaptive CNA isolate dislocations

Conclusion

- **Long Term Goal:**
  - Observe and quantify the behavior of fuel-clad debonding
    - Effects of intermixing and radiation dose
    - Effects of interface structure

- **Short Term Results:**
  - Developed a reliable method of constructing misfit interface
  - Analyzed dislocation network structure of principle crystal planes combinations
  - Confirming with continuum mechanics derived theory
  - Presentation to be given at TMS 2017
  - Manuscript in preparation

Personal: Elton Chen

- Georgia Institute of Technology
- Nuclear & Radiological Engineering B.S. (Ph.D.)
- Research Experience
  - SEM / EBSD (INL)
  - Phonon / DFT (LLNL)
  - Atomistic Simulation / Molecular Dynamics
  - Sample Production / XRD / Texture
- Future Plans
  - Finish Ph.D!