Microstructural Material Modeling (3M) Group research overview

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Degradation of nuclear materials

- Nuclear materials, fuels and structural components, operate in extreme conditions combining high temperature, intensive irradiation, high stress, and corrosion.
- Accordingly, substantial material degradation has been seen including losing of dimensional stability, functional properties, and mechanical integrity.
- This is also a big challenge for materials to be used advanced reactors.

Dimensional stability: e.g., swelling

Functional properties: e.g., thermal conductivity

Mechanical integrity: e.g., fragmentation

L.K. Mansur, JNM 216 (1994) 97-123


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Research mission, approach, and methods

The mission
- Uncover the fundamental mechanisms that are responsible for materials degradation
- Predict the in-service degradation rates of fuels and materials in nuclear reactors
- Aid in developing advanced and materials for applications in extreme environment

The approach: Microstructure-based modeling to establish the PSPP correlations

The method: Multiscale modeling and simulation

In close synergy with experiments.


G.B. Olson, Science (1997)
Current project 1: Statistical modeling of the effect of microstructural heterogeneity on the irradiation behavior of TRISO fuel buffer layer

“TRISO Particles: The Most Robust Nuclear Fuel on Earth”
---U.S. Department of Energy

- **Applications:**
  - High temperature gas-cooled reactor
  - Molten salt reactor

- **Advantages**
  - “TRISO particles cannot melt in a reactor”
  - Withstand extreme environment
  - Retain fission products

- **Industry**
  - INL/EPRI
  - X-Energy
  - Kairos

https://x-energy.com/fuel/triso-x

Current project 1: *Statistical modeling of the effect of microstructural heterogeneity on the irradiation behavior of TRISO fuel buffer layer*

Yet, it still fails, although with an extremely low rate

Hypothesis:
This is caused by the difference in the initial pore structure

Q: Why different crack behavior?
Current project 1: *Statistical modeling of the effect of microstructural heterogeneity on the irradiation behavior of TRISO fuel buffer layer*

**Proposed research**

- Experimental characterization of initial buffer pore structure (UW, ORNL)
- BISON statistic modeling of fracture with various initial pore structure (UW, INL)
- Lower-length scale modeling to supply materials properties (UW, TAMU)
Current project 1: buffer tearing in TRISO fuel

• **Sponsor:** DOE, NE, Nuclear Energy University Program
  ➢ Advanced Gas Reactor Program

• **Collaborators**
  ➢ UW: Professors Kumar Sridharan and Ramathasan Thevamaran
  ➢ TAMU: Professor Karim Ahmed
  ➢ ORNL: Dr. Tyler Gerczak
  ➢ INL: Dr. Wen Jiang
  ➢ Idaho State University: Professors Daniel LaBrier and Mary Lou Dunzik-Gougar

• **Funding amount**
  ➢ $800K (~$260K to our group)

• **Funding period**
  ➢ 10/1/2020-9/30/2023
Current project 2: **HIP Cladding and Joining to Manufacture Large Dissimilar Metal Structures for Modular and GEN IV Reactors**


- **Applications:**
  - Small-modular reactors
  - Gen-IV reactors

- **Advantages:**
  - Simplified fabrication
  - No welding

- **Industry**
  - INL/EPRI
  - GE
  - Westinghouse
  - SynertechPM

Q: What happens at the interface: interdiffusion, phase transformation, etc.?
Current project 2: HIP Cladding and Joining to Manufacture Large Dissimilar Metal Structures for Modular and GEN IV Reactors

Proposed research: Formation of interaction zone between dissimilar metals

- AU/EPRI: Establish a general standard practice for robust HIP based manufacturing for dissimilar metal cladding and joining;
- UW: Create HIP modeling tools
- Develop the understandings of feedstock powder quality control;
- Evaluate the long-term risk of material degradation due to thermal aging and corrosion

Moose phase field modeling of interaction zone between UMo and Zr
Current project 2: HIP Cladding and Joining to Manufacture Large Dissimilar Metal Structures for Modular and GEN IV Reactors

• **Sponsor**: DOE, NE, Nuclear Energy Enabled Technology

• **Collaborators**
  - Auburn: Professor Xiaoyuan Lou (lead PI)
  - EPRI: Drs. David Gandy, Stephan Tate
  - GE: Drs. Raul Rebak, Fran Bolger
  - Westinghouse: Clinton Armstrong
  - Synertech PM: Victor Samarov

• **Funding amount**
  - $1,000K (~$180K to our group)

• **Funding period**
  - 10/1/2020-9/30/2023

• **Remarks**: We are interested in mesoscale modeling of interdiffusion, reaction, and phase transformation. These techniques will be applicable for molten salt corrosion of alloys.
Current project 3: The Role of Anisotropy on the Self-Organization of Gas Bubble Superlattices

Irradiation not always causes damages, it creates artistic nanoscale patterns

Self-organization of nanoscale void and gas bubbles superlattices have been observed in many fcc and bcc metals and alloys. Combining rate-theory based instability analysis and kinetic Monte Carlo and phase field simulations, we have successfully explained superlattice formation based on 1D interstitial diffusion. Still, question exist on how superlattice form in fcc metals where interstitial perform 3D diffusion?
Current project 3: The Role of Anisotropy on the Self-Organization of Gas Bubble Superlattices

Hypothesis: Superlattice form in fcc metals and bcc Fe due to 1D diffusion of interstitial clusters such as loops.

Proposed research:

- **UW**: Further development of the atomic kinetic Monte Carlo code to include interstitial formation and diffusion and simulate superlattice formation;

- **INL/BNL**: Superlattice formation in fcc Ni and bcc Fe under gas ion irradiation followed by advanced characterization using HR-TEM and synchrotron beams; phase field modeling of superlattice formation.

AKMC simulation of superlattice
Current project 3: The Role of Anisotropy on the Self-Organization of Gas Bubble Superlattices

- **Sponsor:** DOE, Office of Science, Basic Energy Science
- **Collaborators**
  - INL: Drs. Jian Gan (lead PI), Cheng Sun, Chao Jiang, Larry Aagesen, Andrea Jokisaari
  - BNL: Drs. Lynne Ecker and Simerjeet Gill
- **Funding amount**
  - $800K/year (~$60K to our group)
- **Funding period**
  - 10/1/2020-9/30/2021
- **Remarks:** A proposal on a related topic is under review.
Current project 4: Mitigating irradiation assisted stress corrosion cracking by rapid alloy design

Combining integrated computational materials engineering (ICME), additive manufacturing, and out-of-pile experiments for rapid design of nuclear materials.

ICME exploration (UW)

Additive manufacturing (Auburn)

Out of pile tests (UMich)

Advanced characterization (INL)

Hf Gradient from 0.2 wt.% to 1 wt.%

1.0 wt% Hf

0.8 wt% Hf

0.6 wt% Hf

0.4 wt% Hf

0.2 wt% Hf

SCC test (Auburn)
Current project 4: Mitigating irradiation assisted stress corrosion cracking by rapid alloy design

- **Proposed research**
  - **UW**: Atomic kinetic Monte Carlo and phase field modeling of radiation induced segregation in steels with minor additives, e.g., Hf, Zr
  - Auburn: Additive manufacturing of modified steels with minor additives and stress corrosion cracking test
  - **UMich**: Proton irradiation of additively manufactured steels
  - **INL**: Advanced characterization of irradiation samples for radiation induced segregation and void swelling

Moose phase field simulations of concurrent grain growth and radiation induced segregation

Left: Cr concentration field

Right: Cr concentration cross two boundaries
Current project 4: Mitigating irradiation assisted stress corrosion cracking by rapid alloy design

• **Sponsor:** Idaho National Laboratory, Lab. Directed Research & Development

• **Collaborators**
  - INL: Drs. Daniel Schwen (lead PI), Lingfeng He, Xiang Liu
  - Auburn: Professor Xiaoyuan Lou
  - UMich: Dr. Miao Song
  - U Wyoming: Professor Dilpuneet Aidhy

• **Funding amount**
  - $1,580K (~$160K to our group)

• **Funding period**
  - 1/1/2020-9/30/2021

• **Remarks:** Also in collaboration with Prof. Haiming Wen at Missouri S&T on an NEUP on this topic.
Current project 5: Fundamental defect properties

**Point defects, as the most basic irradiation damage in materials, govern the responses of materials under irradiation**

Combining atomistic calculations such as density functional theory (DFT) and molecular dynamics (MD) simulations, and statistic mechanics, thermodynamic and kinetic properties of point defects and their role in long-term irradiation behavior in concentrated alloys (UMo, UZr, FeNiCr, etc.) are being investigated.

**Vacancy-solute binding**

**Change in elastic moduli in UMo due to point defects**
Current project 5: Fundamental defect properties

• Sponsors: DOE ARPA-E (UZr), DOE NNSA USHPRR program (UMo)

• Collaborators
  ➢ INL: Drs. Michael Benson (lead PI for ARPA-E), Sudipta Biswas, Stephen Novascone
  ➢ PNNL: Dr. Shenyang Hu
  ➢ ANL: Drs. Bei Ye and Zhigang Mei
  ➢ NCSU: Professor Benjamin Beeler (lead PI for HPRR)
  ➢ Oklo: Dr. John Hanson

• Funding amount
  ➢ ARPA-E: $2,000K (~$90K to our group)
  ➢ USHPRR: ~$900/year (~$70K to our group so far)

• Funding period
  ➢ ARPA-E: 1/1/2020-9/30/2021
  ➢ USHPRR: 1/1/2020-9/30/2023

• Remarks: A proposal on this topic is pending
Future projects

• A few areas are being explored for future research
  - Vacancy properties in random, concentrated alloys
  - Self-organization under irradiation (or in other non-equilibrium condition)
  - Phase stability of concentrated alloys under irradiation
  - Moten salt corrosion