INL/MIS-18-51272-Revision-0

Development of a Synergistic Approach to Study Irradiated Materials Using Coupled Experiments and Simulation - FY2018 final poster

Cynthia A Adkins, Assel Aitkaliyeva, Michael Tonks, Daniel M Wachs, Jacob Hirschhorn

August 2018

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Development of a Synergistic Approach to Study Irradiated Materials Using Coupled Experiments and Simulation

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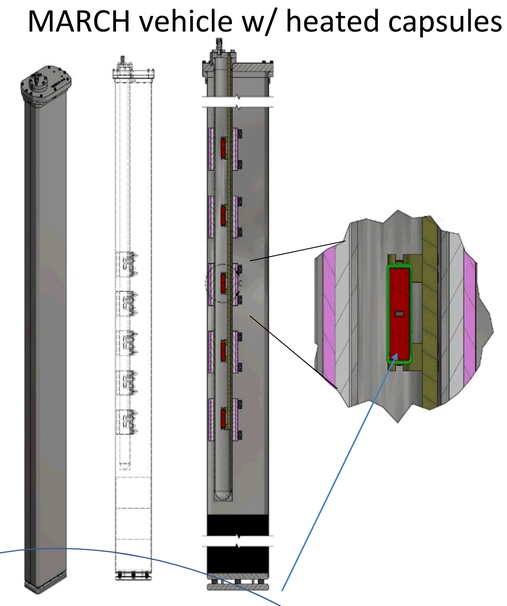
Objective

1) develop experimental procedures to obtain the specific pre- and post-irradiation characterization data required for validation and uncertainty quantification of MARMOT models
2) understand the evolution of microstructure under transient irradiation conditions and its impact on properties for use with TREAT.
3) demonstrate the value of a coupled experimental and simulation approach on understanding critical thermal properties in a material of broad interest (the U-Pu-Zr system and its binaries)

Technical Challenges

- New irradiation hardware design was needed to enable irradiation in TREAT – MARCH vehicle
- TREAT irradiation scheduled for year 2 of this project was delayed

MARCH vehicle w/ heated capsules

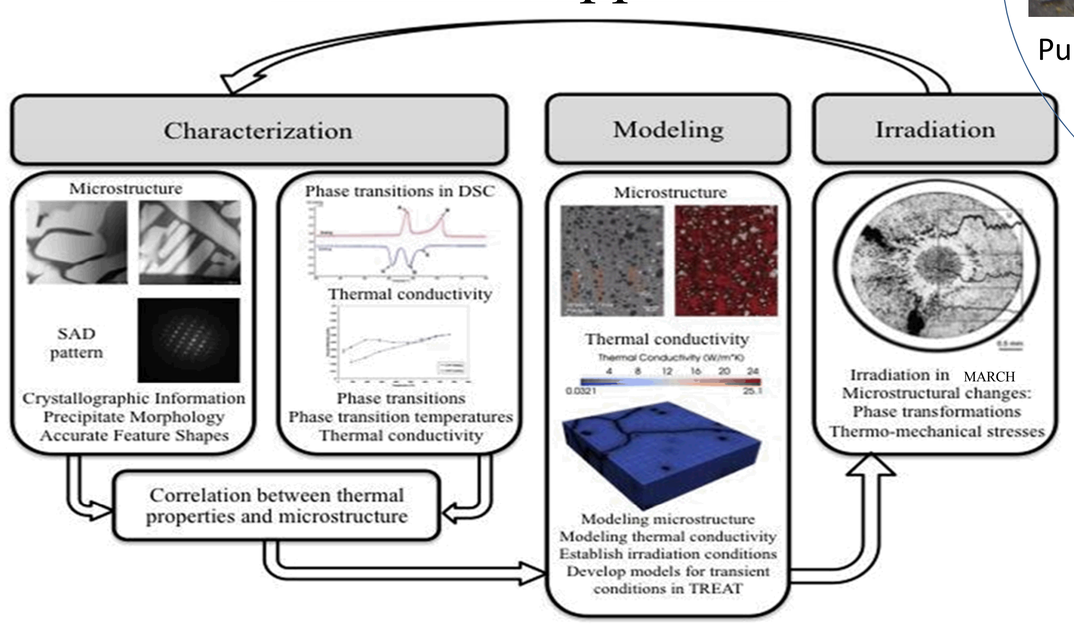


Pu – 30 wt% Zr

U-20 wt% Pu-10 wt% Zr

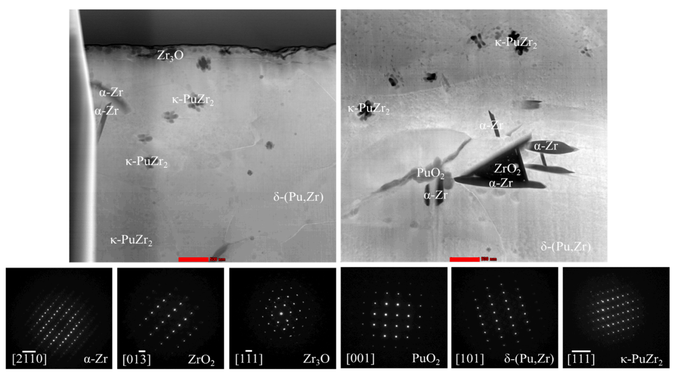
Pu – 10 wt% Zr

Technical Approach

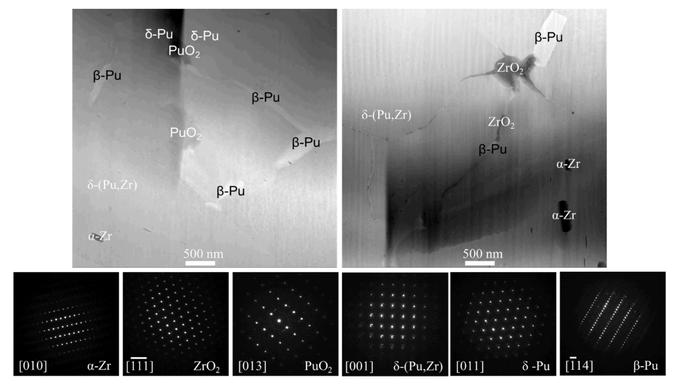


Characterization Results

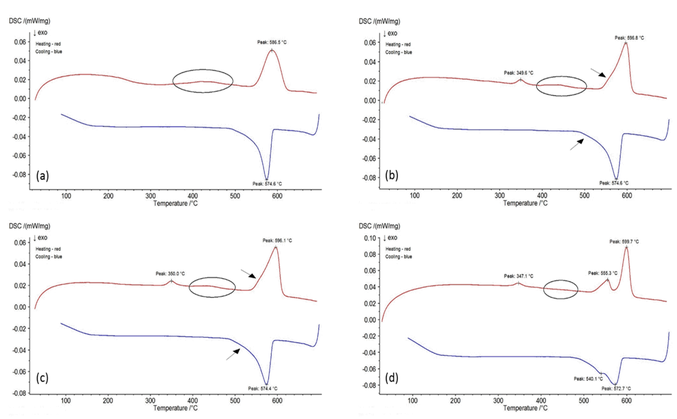
- Microstructure was observed with SEM, TEM and crystal structure determined with SAED patterns (as-cast vs. anneal at TREAT temperature)
- Phase transition temperatures and energies were measured
- Thermal conductivity was measured



Representative phases observed in the as-cast Pu-10Zr specimen. Scale bar denotes 500 nm.



Representative phases observed in the annealed Pu-10Zr specimen. Scale bar denotes 500 nm.



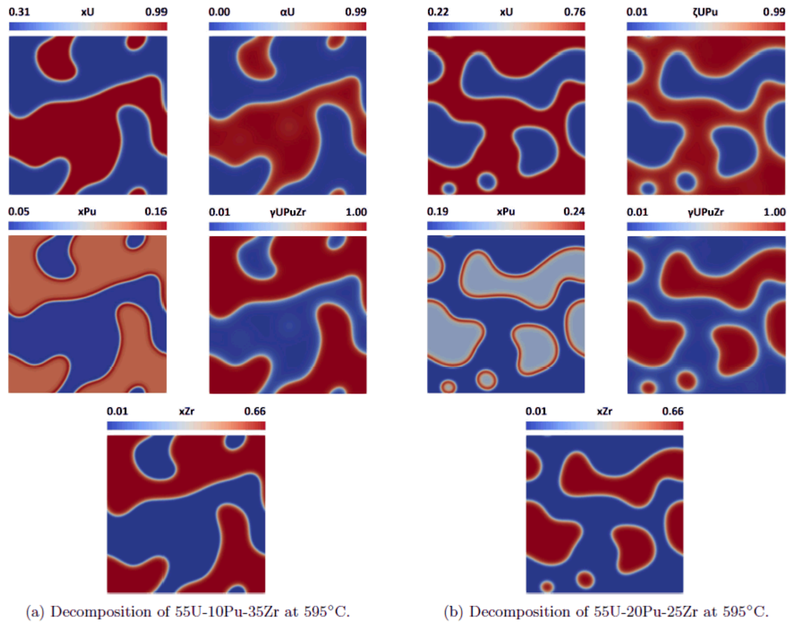
DSC signal vs. Temperature (˚C) for Pu-10Zr upon heating and cooling

(a) 1st thermal cycle of as-cast material (b) 2nd thermal cycle of as-cast material (c) 3rd thermal cycle of as-cast material (d) 1st thermal cycle of annealed material

Modeling Results

- Uses measured and published single phase transition temps to predict microstructure evolution with phase-field model

Phase Transition	x_U	x_{Pu}	x_{Zr}	T_{sim} [°C]	T_{ref} [°C]
$\alpha Pu \rightarrow \beta Pu$	0.00	1.00	0.00	125	125
$\beta Pu \rightarrow \gamma Pu$	0.00	1.00	0.00	214	215
$\gamma Pu \rightarrow \delta Pu$	0.00	1.00	0.00	320	318
$\delta Pu \rightarrow \delta' Pu$	0.00	1.00	0.00	460	463
$\delta' Pu \rightarrow \gamma UPuZr$	0.00	1.00	0.00	480	483
$\zeta UPu \rightarrow \eta UPu$	0.63	0.37	0.00	619	640
$\eta UPu \rightarrow \gamma UPuZr$	0.63	0.37	0.00	704	710
$\alpha U \rightarrow \beta U$	1.00	0.00	0.00	668	668
$\beta U \rightarrow \gamma UPuZr$	1.00	0.00	0.00	776	776
$\delta Pu \rightarrow \gamma UPuZr$	0.00	0.40	0.60	631	630
$\alpha Zr \rightarrow \gamma UPuZr$	0.00	0.00	1.00	864	863
$\delta UZr \rightarrow \gamma UPuZr$	0.30	0.00	0.70	617	610



(a) Decomposition of 55U-10Pu-35Zr at 595°C.

(b) Decomposition of 55U-20Pu-25Zr at 595°C.

Publications

- Development and Verification of a Phase Field Model for the Equilibrium Thermodynamics of U-Pu-Zr, Hirschhorn, Tonks, Aitkaliyeva, Adkins – in review
- The evolution of the microstructure and thermal properties of Pu-10Zr fuels with temperature, Aitkaliyeva, Adkins, Hirschhorn, McKinney, Tonks – in draft
- Thermal Conductivity of Pu-Zr alloys, Adkins, Aitkaliyeva, Hirschhorn, Tonks – in draft
- 9+ presentations in conference proceedings

Harvest Strategy Result

The work completed for this LDRD has attracted interest from the NTRD program in FY 2019 to develop a new work package for separate effects testing

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