Phase Field Modeling of the Tetragonal-to-Monoclinic Phase Transformation in Zirconia

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Introduction

The tetragonal to monoclinic phase transformation (T→M) in zirconia is an important contributor to the failure of nuclear fuel rods used in nuclear power plants. A model of this process has been developed using a phase field method by Mamivand *et al.* Our goal is to apply this model using the MOOSE framework. MOOSE, multi-physics object oriented software environment, is a valuable tool for modeling T→M because:

- Automatic parallelization
- Finite Element Framework
- Plug-n-physics modules
- Free and open source

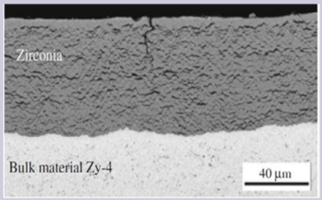

Figure 1. Zirconia cladding crack.

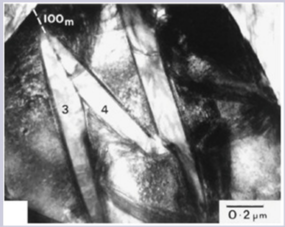

Figure 2. TEM micrograph of partially transformed t-ZrO_2.

Objectives

- Understand MOOSE framework and it's phase field module.
- Learn phase field method of martensitic T→M in zirconia.
- Implement the T→M of zirconia into MOOSE.

Methods

- Phase Field Equations
- Material Properties
- Energy Functions

→ MOOSE Input File for Processing

Phase Field Method:

- Mathematical model used for moving boundary problems.
- Minimizes and accounts for all the energies.
- Ginzburg-Landau Kinetic Equation implemented into MOOSE kernels to define the phase field model:

$$\frac{\partial \eta_p(\boldsymbol{r},t)}{\partial t} = -L\frac{\delta F}{\delta \eta_p(\boldsymbol{r},t)}, p = 1, \ldots$$

```
[Kernels]
  [./eta_bulk1]
    type = AllenCahn
    variable = eta1
    args = 'eta2'
    f_name = F
  [../]
```

MOOSE

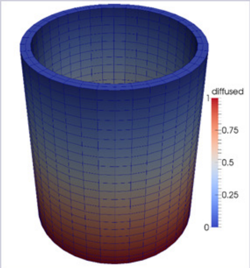

Figure 3. MOOSE code utilizes coupled and implicit multi-physics solvers to calculate solutions which can be viewed using the built in GUI, Peacock.

Results

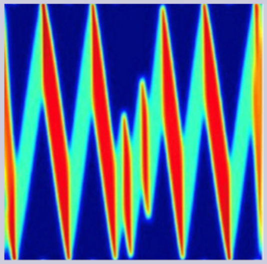

Figure 4: Zirconia T→M using COMSOL.

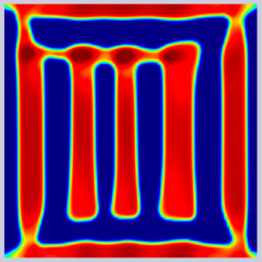

Figure 5: Current results using MOOSE.

Conclusion

MOOSE is capable of modeling T→M in zirconia with an approach more valuable than classical methods. This could provide important insight for development of nuclear fuel rods for prevention of cracking.

Future Works

Figure 6. Falcon Supercomputing System located at INL.

- Continue fixing parameters in MOOSE to represent T→M zirconia structure as shown in figure 2.
- Run MOOSE code on the supercomputer at Idaho National Lab to generate large quantities of data.
- Apply machine learning and AI algorithms to accumulated data for further elucidation.

[1] Mamivand, M., Zaeem, M. A., Kadiri, H. E., & Chen, L. (2013). Phase field modeling of the tetragonal-to-monoclinic phase transformation in zirconia. Acta Materialia,61(14), 5223-5235. doi:10.1016/j.actamat.2013.05.015
[2] Brian Alger and David Andr and Robert W. Carlsen and Derek R. Gaston and Fande Kong and Alexander D. Lindsay and Jason M. Miller and Cody J. Permann and John W. Peterson and Andrew E. Slaughter and Roy Stogner. (2019). MOOSE Web Page, https://mooseframework.org
[3] Derek R. Gaston and Cody J. Permann and John W. Peterson and Andrew E. Slaughter and David Andr and Yaqi Wang and Michael P. Short and Danielle M. Perez and Michael R. Tonks and Javier Ortensi and Ling Zou and Richard C. Martineau. (2015). Physics-based multiscale coupling for full core nuclear reactor simulation, Annals of Nuclear Energy.
[4] Mamivand, M., Zaeem, M., Kadiri, H. Phase Field Modeling of Tetragonal to Monoclinic Transformation in Zirconia. Mississippi State University

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