Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program
Fundamental Methods and Models (FMM)

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FMM Objectives

- Provide cross cutting fundamental material and chemistry models to various IPSCs
- Develop lower scale and mesoscale methods and capabilities
- Provide upscaling methods from atomistic to continuum including propagation of uncertainty in scales.
- Provide single point of contacts for IPSCs
- Collect requirements from IPSCs
- Work with VU to validate and verify lower scale and upscaling methods.
- Provide interactions with NEUP projects
- Provide benchmark and comparison of various modeling techniques at various scales for various phenomena

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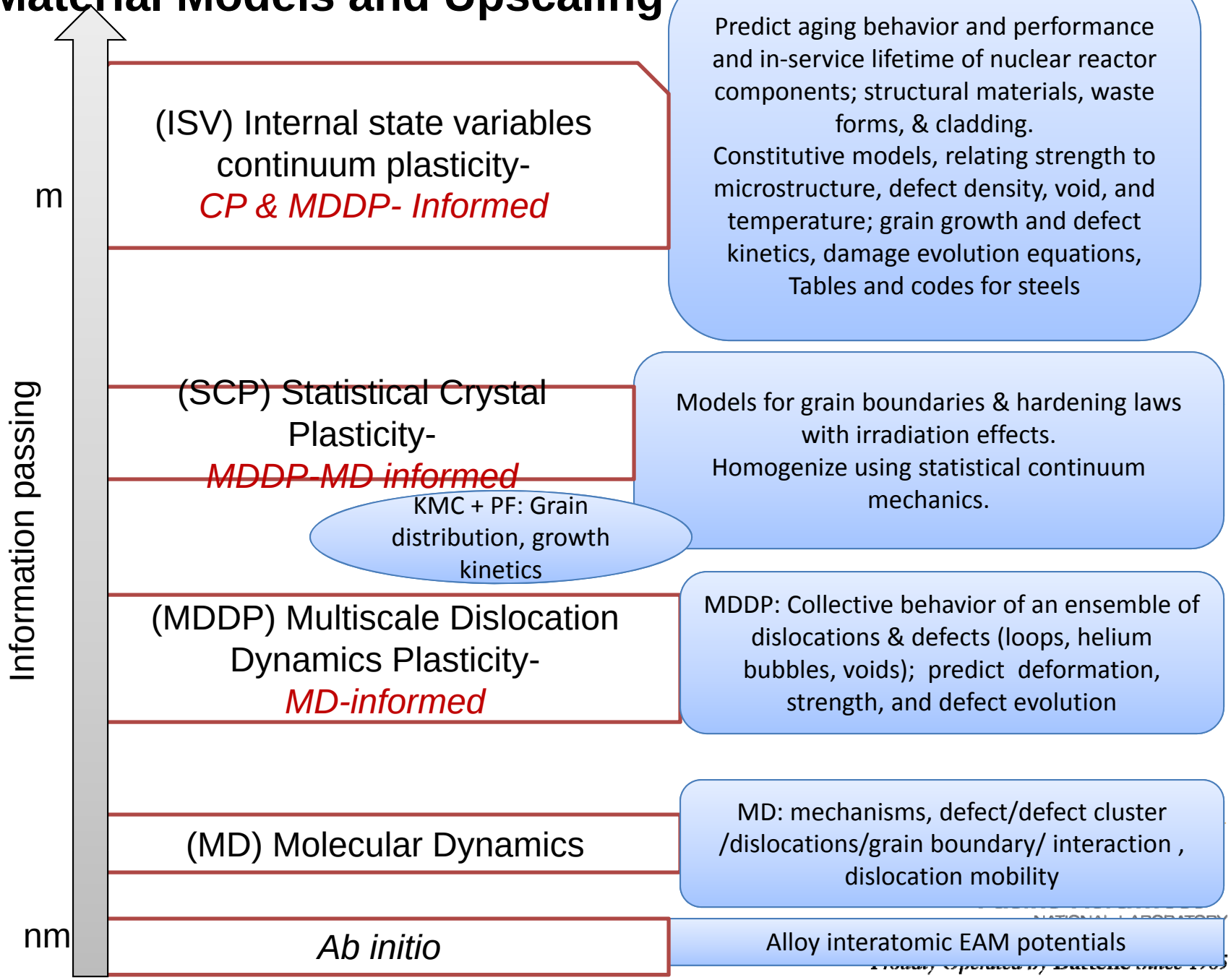
Material Models and Upscaling



Highlights of FY10 Accomplishments

- PNNL
  - Delivered report entitled Fundamental Science-Based Simulation of Nuclear Waste Forms (FCR&D-MDSM-2010-00168).
  - Obtained accurate defect formation energies in the nuclear waste form ceramic, xenotime (YPO_4), using density functional theory, developed several interatomic potentials for xenotime (YPO4) to use in classical molecular dynamics simulations, and developed preliminary protocols based on lattice constants, elastic constants and thermal expansion to validate the interatomic potentials.
  - Developed a phase-field model to simulate void migration in a temperature field and volume swelling under nuclear irradiation, and the growth kinetics of interstitial loop in irradiated materials

Highlights of FY10 Accomplishments

- PNNL
  - Developed stress-strain curves maps, and defect evolution during plastic deformation in pure alpha-Fe using large scale DD simulations with input from MD. Developed constitutive laws for the flow stress and its dependence on both defect density and dislocation density, also developed an evolution for the defect density during plastic deformation.
  - Developed a multiscale model to predict microstructure and thermal conductivity evolution of polycrystalline materials during irradiation by bridging phase field model and statistical continuum mechanics model.

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Highlights of FY10 Accomplishments

- ORNL
  - Developed a framework for modeling NpO2-x and incorporated that into a prospective (U,Pu)O2 thermo-chemical model.
  - Provided volume fraction and distribution of gas bubbles within the microstructure as a function of grain size, temperature and gas (Xe and Kr) production rate to the macroscopic code.

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Highlights of FY10 Accomplishments

- Sandia
  - Delivered 2 reports: “Upscaling Atomistic Mechanisms to Continuum Models For Nuclear Waste Glass Dissolution” and “Development of a Hybrid Potts – Phase Field Method”
  - Development of a Hybrid Potts – Phase Field Method;
  - Upscaling Atomistic Mechanisms to Continuum Models For Nuclear Waste Glass Dissolution
- LANL
  - Finalizing the fission cross-section calculations for a complete suite of plutonium isotopes
- LLNL
  - Completed Pu and Am pseudopotential for the ABINIT software tool

Collaborations with Other Program Elements

- Fuels IPSC: established collaboration on the development and validation of mesoscale material methods (INL, LANL, PNNL), (SNL, ORNL)
- Waste Form IPSC: systematic approach for developing interatomic potentials (SNL, PNNL)
- VV&UQ: Protocols for VQ for fine scale and upscaling (SNL, PNNL)
- Safe Seps: established new activities for chemistry models (LANL, PNNL, SNL)

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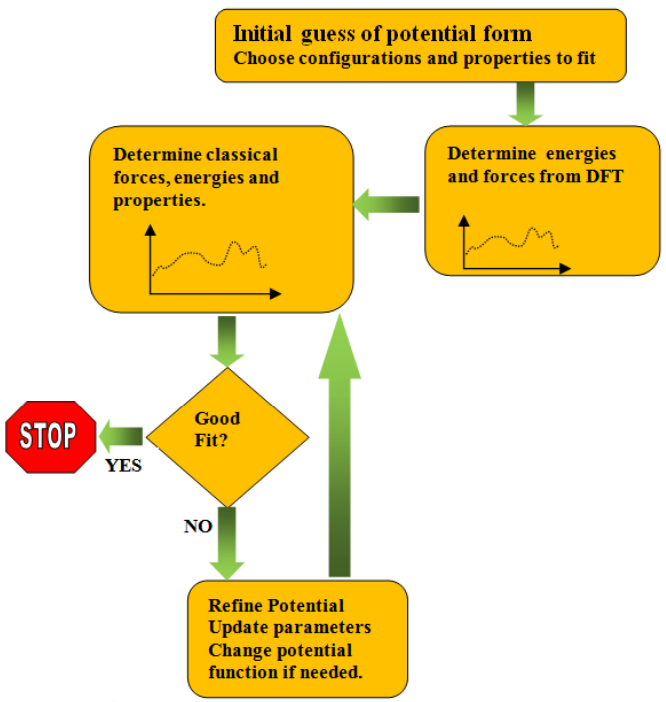
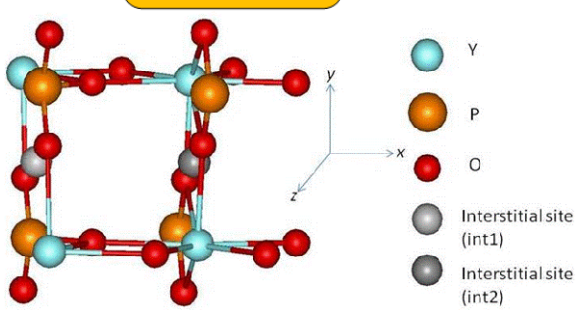
Interatomic potential development for a waste form

We have developed an interatomic potential for a durable waste form, YPO_4. We will refine the potential based on our DFT data shown below.

METHOD





RESULTS

Property	Potential	Experiment
Lattice constant *a* (Å)	6.895	6.883
Lattice constant *c* (Å)	6.029	6.021
C_{11} (GPa)	220	220
C_{12} (GPa)	28	55
C_{13} (GPa)	93	86
C_{33} (GPa)	337	332
C_{44} (GPa)	65	65
C_{66} (GPa)	17	17

Sample defect formation energies from DFT

Defects	Formation energy (eV)
Vacancies	
Y_{vac}	15.09
P_{vac}	17.94
O_{vac}	14.29
Antisite defects	
Antisite pair	12.66
Y_P	6.22
P_Y	10.06

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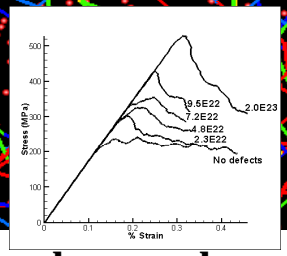
Hierarchical Multi-scale Modeling of Irradiation Induced Strengthening

H. Zbib, D. Field, I. Mastorakos (WSU), Hamid Garmestani (GT)
M. Khaleel, X. Sun, D. Li, R. Devanathan (PNNL)

Objective: Develop a physically-based capability that predicts aging behavior & performance, & in-service lifetime of nuclear reactor components with emphasis on structural materials



Outcomes/Benefits

Mulit-scale models and methods to predict strength and damage evolution laws for use in the integrated codes.

Fundamental

The effect of irradiation on materials microstructure and mechanical properties is an inherently multi-scale phenomenon involving processes spanning a wide range of length and time scales.

Approach and Research Strategy

Multiscale models and methods based on **information passing** between length scales

Accomplishments

Molecular Dynamics

Developed: mechanisms, defect/defect cluster /dislocations/grain boundary/ interaction , dislocation mobility

Crystal plasticity

Developed method & models: hardening laws, including effect of defect clusters & grain boundaries

Dislocation Dynamics

Performed large scale simulations of ensemble of dislocations & defects; and

Developed models: deformation, strength, and defect evolution

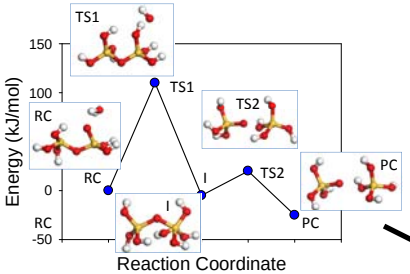
continuum plasticity

Predict aging behavior and in-service lifetime of nuclear reactor components

Gap Analysis on Modeling Aluminosilicate Dissolution

FY10 FMM & Waste IPSC – Louise Criscenti (SNL)

Atomic/Quantum



Ab initio cluster calculations to determine bond-breaking energies

Gap 1

❖No consensus on how activation energies for bond-breaking should be modeled in cluster calculations

❖Not clear how to go from the energy of breaking one bond to dissolving "crystal units"

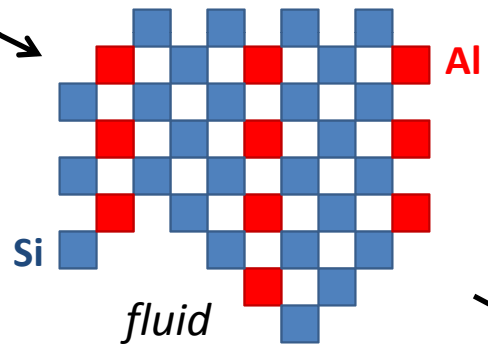
Gap 2

❖Mesoscale models are used to test dissolution scenarios – not completely predictive.

❖Not clear how to link mesoscale models directly to continuum models or develop new constituitive equations from them.

"Mesoscale"

Gap 1



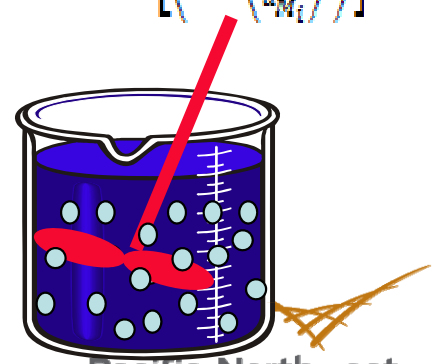
Stochastic Monte Carlo Modeling of the dissolution and re-precipitation of crystal units SiO_4 and AlO_4

Constitutive equations developed to fit leach data from bulk experiments.

Continuum

$$r = k \prod_{i=1, i\neq k}^{i} \left[\frac{K_i \left(\frac{a_{H^+}^{v_i}}{a_{M_i}^{v_i}} \right)^s}{\left(1 + K_i \left(\frac{a_{H^+}^{v_i}}{a_{M_i}^{v_i}} \right)^s \right)} \right]$$

Gap 2



Gap 3

❖Aluminosilicate crystal dissolution → Nuclear Waste Glass Dissolution

Speakers

- Hierarchical Multi-scale Modeling of Irradiation Induced Strengthening – Professor Zbib (WSU)
- F-electron Problem: Approach to Improving Accuracy of Density Functional Theory for Actinide Materials – Anne Mattsson (SNL)
- Molecular Dynamics and Meso-scale Modeling Framework for Irradiation Damage - Ram Devanathan and Xin Sun (PNNL)

Looking Ahead – 6 FMM Focus areas

- **Models (material properties)**: Developing a mechanism-based capability to predict aging behavior and performance of nuclear reactor components with emphasis on structural materials and cladding
- **Models (material microstructure):** Developing state-of-the-art methods and applying those methods to develop models of irradiated microstructures, defect distributions and kinetic laws of defect growth and evolution for Fuels (Cladding), Reactor (Structural Materials), and Waste Forms (Stability) IPSCs.
- **Models (chemistry):** Developing methods to predict thermodynamics properties of actnidies and fission products in a wide range of temperature and pressure and developing reliable tools to predict the properties of liquids, solvation and kinetics in solutions

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Looking Ahead – Methods

- **Methods (lower scales)**: Developing integrated methods (ranging from density functional theory (DFT), classical molecular dynamics (MD) simulations to long term dynamics and kinetic Monte Carlo simulations) to model the behavior of waste form and structure materials and determining basic physics information for mesoscale and sub-continuum models
- **Methods (mesoscale):** Upscaling prediction models from microscale to mesoscale by phase field model, including a proof-of-principle and illustrative simulation. Coupling kinematic Monte Carlo with phase field model to reach a mechanistic understanding of coupled chemistry-microstrucutre evolution phenomena, relevant to Fuels, Wasteforms, and, possibly, Safe Separations IPSCs
- **Methods (atomistic->continuum):** Linking atomistic results to continuum models by developing methodologies to “roll up” quantum or classical atomistic information into “bulk” properties or developing new continuum constitutive equations, including methods to determine likely reaction mechanisms.

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Questions and suggestions?