NEUP Nuclear Energy University Programs

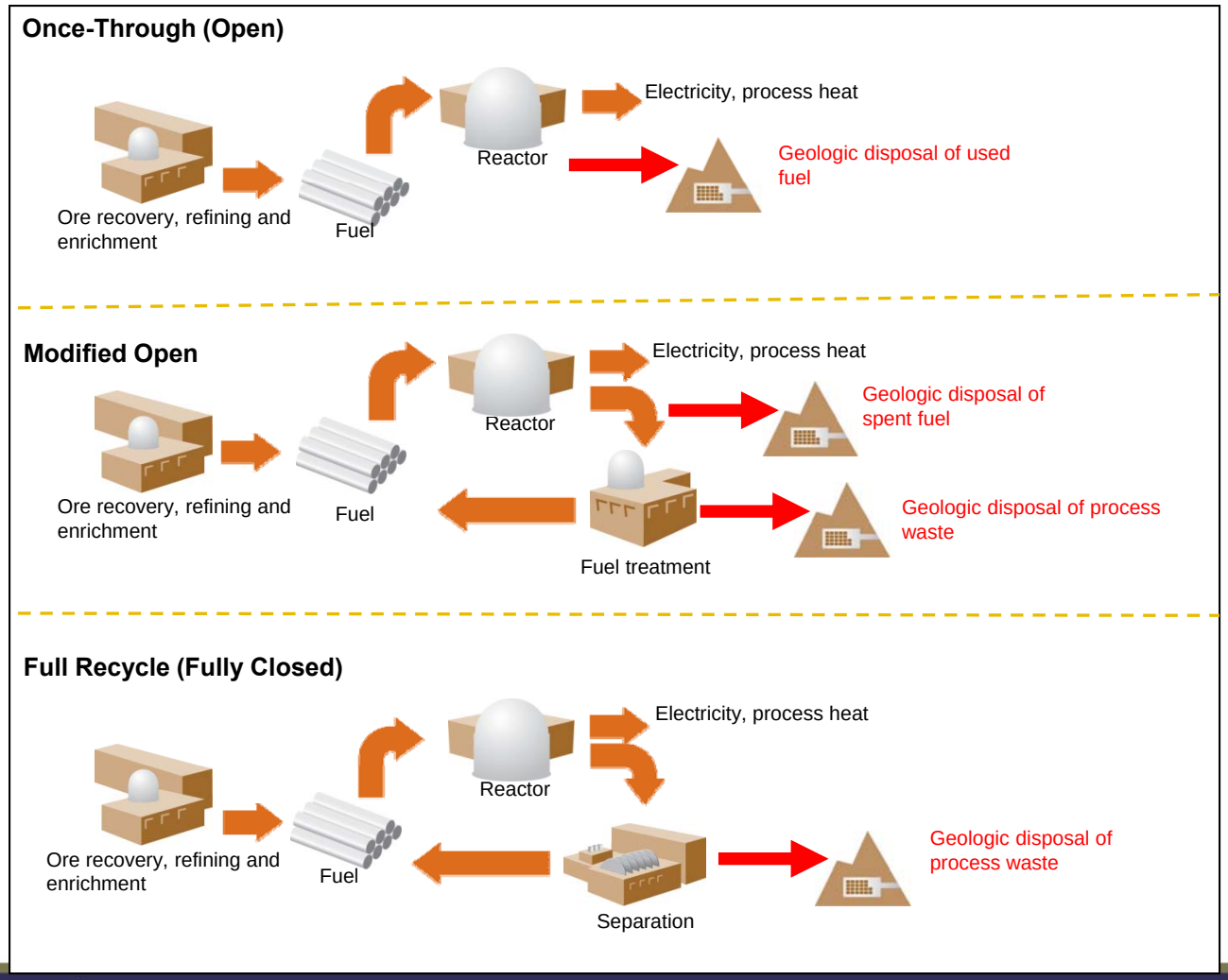
U.S. Department of Energy

July 27-28, 2010

FY2011 NEUP Workshop Materials (M) Breakout Session

Rockville, Maryland

Fuel Cycle Research and Development



Once-Through – One pass through reactor, directly disposed in a geologic repository.

Modified Open – Limited separations and processing applied to used fuel to extract more energy.

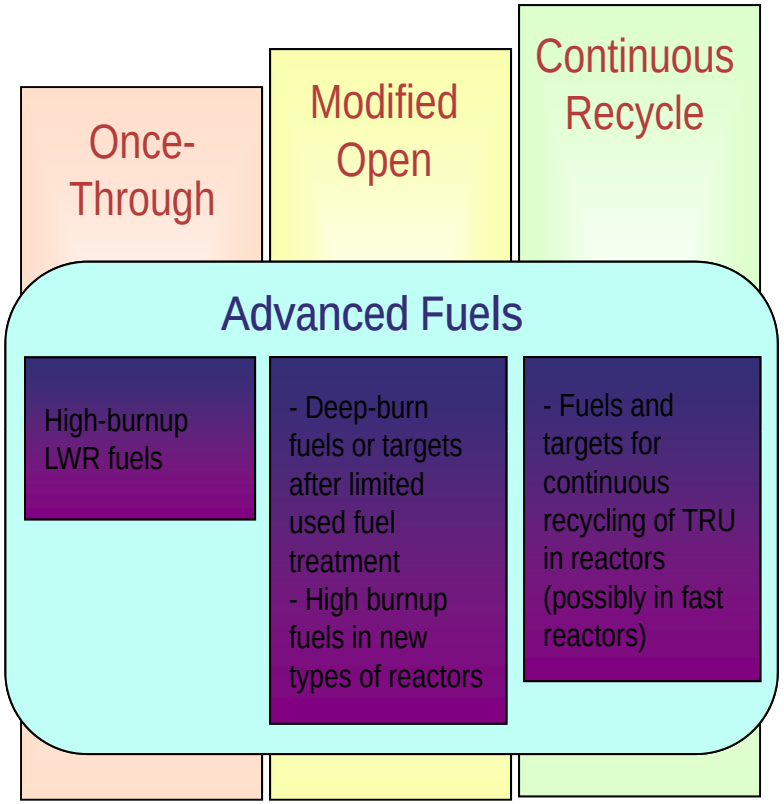
Full Recycle – All actinides important for waste management are recycled in thermal or fast spectrum systems to reduce radiotoxicity and more fully utilize uranium resources.

Advanced Fuels Campaign Mission & Objectives

- Mission

  Develop and demonstrate fabrication processes and in-pile performance of advanced fuels/targets (including the cladding) to support the different fuel cycle options defined in the NE roadmap.
- Objectives

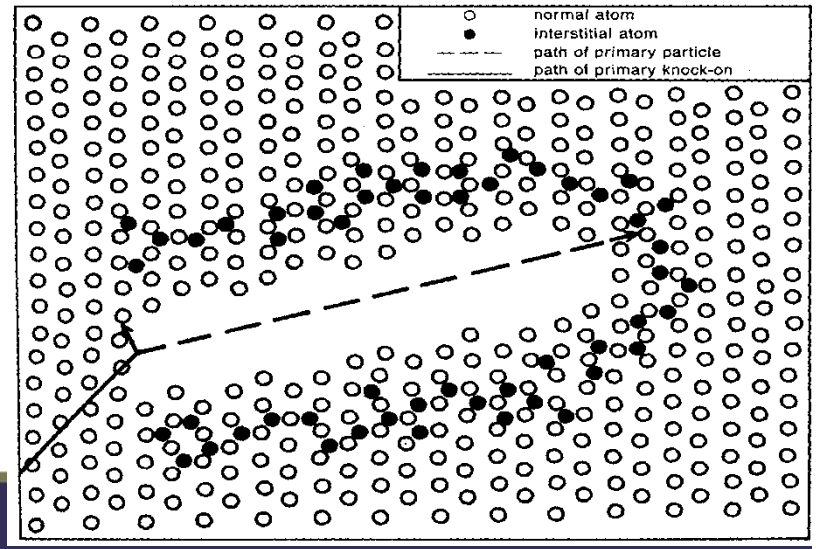
  Development of the fuels/targets that
  - Increases the efficiency of nuclear energy production
  - Maximize the utilization of natural resources (Uranium, Thorium)
  - Minimizes generation of high-level nuclear waste (spent fuel)
  - Minimize the risk of nuclear proliferation
- Grand Challenges
  - Multi-fold increase in fuel burnup over the currently known technologies
  - Multi-fold decrease in fabrication losses with highly efficient predictable and repeatable processes



Grand Challenge for Core Materials to Enable Multifold Increases in Burnup for Fuels

- Develop and test advanced alloys suitable for clad and duct and other high dose core components to >400 dpa over the clad /duct operating conditions
  - Irradiation tolerant
    - Resists swelling and creep
    - Does not accumulate damage (resists hardening and embrittlement)
    - Stable microstructure (resists radiation induced segregation)
    - Manages helium or other gas buildup
    - Stable with Transmutation impurity buildup
  - Resist chemical interaction with fuel

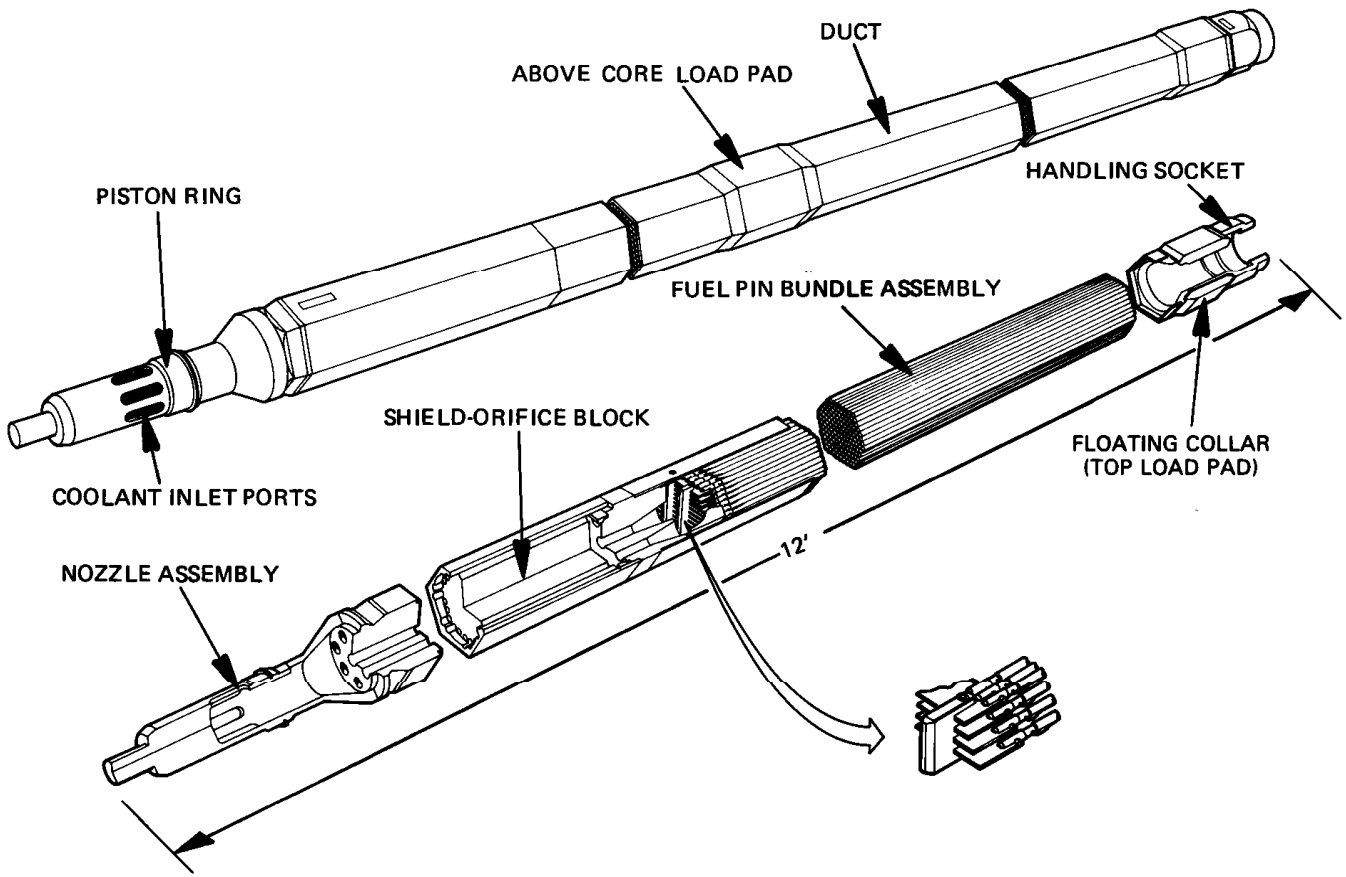
  (for the cladding)
    - Not reactive with fuel
    - Prevent diffusion into cladding
  - Corrosion resistance with coolant
    - Protective oxide layer
    - Non reactive with coolant
  - Weldable and Processed into tube form



Fast Reactor Clad and Duct

- Fast reactor fuel pin cladding is typically ~7 mm diameter by 0.5 mm wall thickness tubing that is used to encapsulate cylindrical fuel pellets.
- Fuel pin length varies with reactor design, usually several meters long.

- **Groups of fuel pins (typically 50-80) are placed into a duct.**
- **The ducts provide mechanical support, segments the core, and forces coolant over the fuel pins.**
- **Typical dimensions are 3 mm thick material with a flat-to-flat distance of ~150 mm**



Materials Challenges for Fast Reactor Clad and Duct

Desirable properties

•High thermal conductivity (allows lower fuel temperature)

•Compatible with fuel (esp. for metal fuels)

•Compatible with coolant (typ. sodium)

•Sufficient strength and ductility

•Thermal creep resistance (allows higher coolant ΔT through the reactor -> greater thermal efficiency for power)

•Physical and mechanical properties immune to irradiation

•Affordable

Irradiation damage effects

- Destruction of "engineered" microstructure
- Increase in thermal conductivity
- Increase in yield strength (unneeded benefit)
- Decrease in ductility and toughness at lower T_m
- Void swelling at intermediate T_m
- Irradiation enhanced creep at intermediate T_m
- Helium embrittlement at higher T_m

Other degradation processes of concern

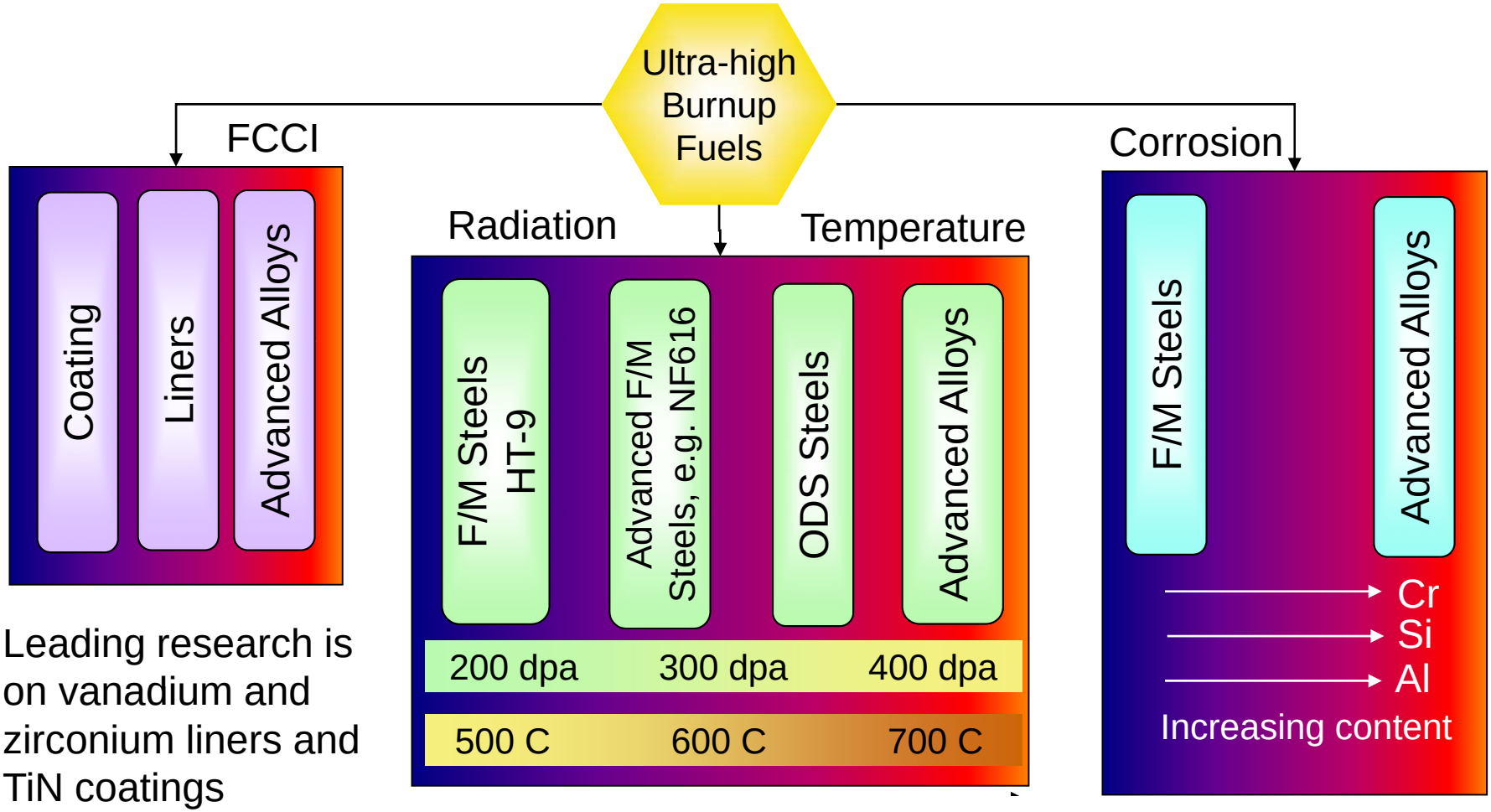
- Thermal creep
- Corrosion due to interaction with sodium coolant
- Fuel cladding chemical interaction (FCCI)

Practical aspects

•Trade-offs in properties have thus far been unavoidable

•Prioritization of desired properties

Achieving the Fuels Grand Challenge – Multifold increases in fuel burnup



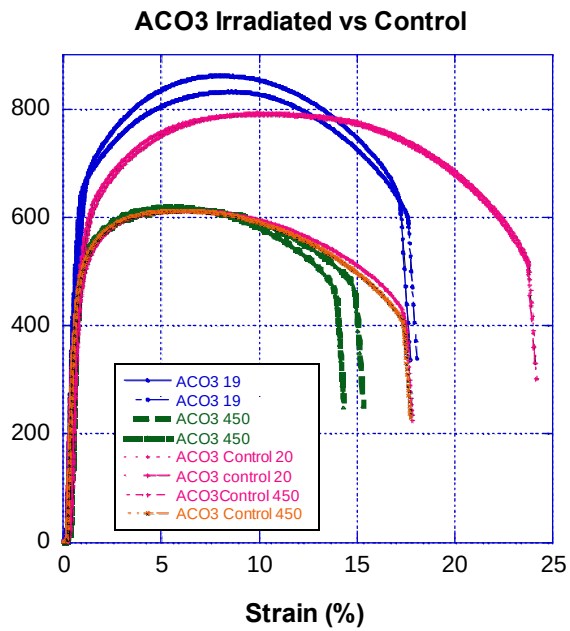
Leading research is on vanadium and zirconium liners and TiN coatings

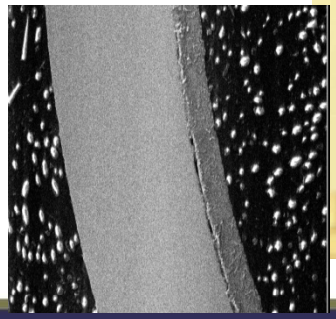
Leading research is on testing highly irradiated HT-9 and T91 (out to 200 dpa). New development efforts on fabricating large heats of ODS alloys (14YWT)

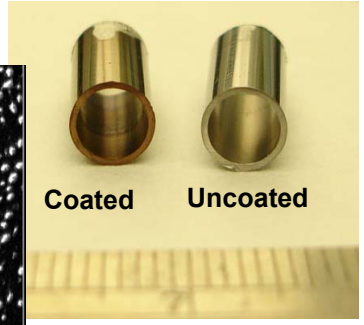
Small studies underway on sodium corrosion testing of F/M steels

Research to Support the Grand Challenges-Core Materials Development

- Knowledge base up to 200 dpa high-dose core materials irradiation data
  - ACO-3 duct testing
    - Fracture toughness testing
    - Charpy testing
    - Tensile testing
    - Tensile testing SANS measurements
  - FFTF/MOTA Specimens and Testing
- Advanced Materials Development
  - Coating/liners to mitigate FCCI
  - Develop and test advanced cladding materials
    - Ion irradiations
    - Testing MA-957 after high-dose irradiations
    - Improved processing of Advanced ODS alloys







Coordinating with Multi-scale Modeling of Radiation Damage in Ferritic Steels

- **Diffraction:** e.g. x-ray, neutron diffraction for defect geometry
- **Spectroscopies:** e.g., NMR, PAS for defect energies, concentration
- **In-situ TEM:** TEM interfaced with ion accelerators for microstructural evolution

Atomistic methods

- First principles calculations
- Semi-Empirical (EAM,MEAM) potentials
- Accelerated dynamics methods

Kinetic Monte Carlo

- Stochastic event based simulation
- Parameterised by atomistic calculations and experiments

Continuum Viscoplasticity Model

- Model for rate-dependent plasticity
- Stress-strain response of polycrystal
- Input from MD/KMC: bubble density, pressure

- **Mechanical Testing** - 3 pt. bend, tensile, shear punch and compression to obtain stress-strain curves

Materials Integration and University and International Collaborations

- Integrate FCRD Materials Activities
  - Fuels Core Materials Work- (INL, PNNL, LANL, ORNL)
    - Materials updates monthly
  - University Materials Research (attend university review, review quarterly progress reports)
  - ATR Reactor Irradiations (provide materials and will collaborate in testing)
  - US-European collaborations
    - INERI-DEMETRA- completed-
    - INERI-GETMAT-
      - Member of User Group
      - INERI in place
- Working group meetings and Workshops
  - Advanced Materials Working Group Meeting held jointly with Structural Materials, J. Busby – UCSB- March 23-25, 2010 – goal –Draft Level 1 report on "Potential Alloy Development to Meet the Grand Challenge"
    - Labs- PNNL, INL, LANL, ANL
    - DOE
    - Universities- UCSB, TAMU, UCB, UMich, PSU, UIUC…
  - Coordinated Materials Meeting – ORNL – July 18-22, 2010
  - Innovative Materials Immune to Radiation Workshop by invitation
    - Vail, CO, August 22-26, 2010
    - Keynote lecturers Karl Whittle-ANSTO-Australia - Rad Eff. in Ceramics; Julia Greer- Cal Tech - Small Scale Testing; John Lewandowski- CWRU- Bulk Metallic Glasses; Arthur Motta- Penn State U. - Rad Effects in Metals; A. Kimura- Kyoto U. - Nano-strengthened Steels; W. Knabel- Plansee- Refractory Alloys; Robin Grimes - Imperial College - Innovative ceramics for rad. Tolerance; Y.W. Kim - UES Inc. - Titanium Aluminides for Aerospace applications

Workscope Description(s)

Development of New Materials (M-6)
RC-ARC:

•Advanced reactor systems - high temperature liquid metal, high temperature molten salt, and other advanced reactor applications.

• Scope of Project

- •Assessment of the advanced material
- •Evaluation of the impact of the material on reducing the cost of an advanced reactor system, improving safety, and other benefits.
- •Evaluation of microstructure stability of advanced structural materials must be validated for fast reactors at elevated temperatures and extended lifetimes.
- •Semi-empirical modeling of fast reactor structural material aging and irradiation degradation mechanisms need to be developed to predict high neutron fluence and temperature effects and bulk/macrostructural mechanical properties, including yield strength, creep, fatigue, ductility, etc., as a function of time, temperature, irradiation damage, and pressure history.
- •Validation and verification of the micro-structural stability of advanced structural materials operating at high temperature, high neutron damage conditions for extended operating lifetimes for anticipated fast reactor operating conditions.
- •Thermal aging and stability tests are needed to assess candidate alloys and must be closely coordinated with advanced alloy development.
- • The university team will develop a structural material lifetime model and create a predictive computer code. This model will be extensively validated by comparison to existing reactor operating data and existing materials tests. This model will capture fluence and temperature effects, but is not anticipated to be atomic level detail.

Workscope Description(s)

Development of New Materials (M-6)
NEET-XAMM and XRM:

- Research new classes of alloys and materials, not yet considered for reactor performance that may enable transformational reactor performance.
- Custom design of innovative steels using modern materials science techniques, industrial knowledge, and previous experience aim to
    - Improve performance over traditional materials by a factor of five to ten,
    - Increasing the maximum operating temperature by 200 degrees Celsius for a period of at least 80 years.
- Concepts that may be evaluated include
    - optimized alloy composition,
    - engineered microstructures,
    - age-tempered microstructures, or combinations thereof.
    - Other, include bimetallic layers, metal/ceramic composites, ion-beam or surface-modified alloys.
    - General goal is improved strength and radiation resistance.

Workscope Description(s)

Materials Modeling (M-8)
NEET-AMS:

- Development of validated materials models and methods that lead to accurate continuum simulations of materials response, with appropriate quantitative consideration of uncertainties at every scale. Examples include:
  - Predictive Models for Material Degradation at Different Scales. Aging and degradation mechanisms of different structural materials under various thermal and irradiation environments need to be better understood, quantified, and validated. Key university research needs in this area include
    - (1) Development of atomistic chemical kinetics parameters and upscaling into meso-scale models;
    - (2) Meso-scale models of microstructural and chemical evolution (e.g., phase field, Potts model, kinetic Monte Carlo and rate theory) with extraction of physical parameters for continuum scale materials models;
    - (3) Validated prediction of physical/mechanical property degradation, i.e., thermal conductivity, yield strength, ductility and fracture toughness, creep resistance, etc., to populate continuum scale constitutive models.
  - To aid in validation of these complex models, Small-Scale Separate Effects Experiments for Model Validation. This element calls for the linkage between model development and small-scale experiments. Small scale separate effect experiments are necessary specifically targeted to validate models for different phenomena at various scales.
  - In addition, methodology development is required for Scale Bridging. Multi-scale approaches (from atomic-level to meso-scale to continuum and from picoseconds to years) are needed. New algorithms to achieve upscaling are a key component to the development of integrated reactor performance and safety codes.