Session IV: FES Materials Damage

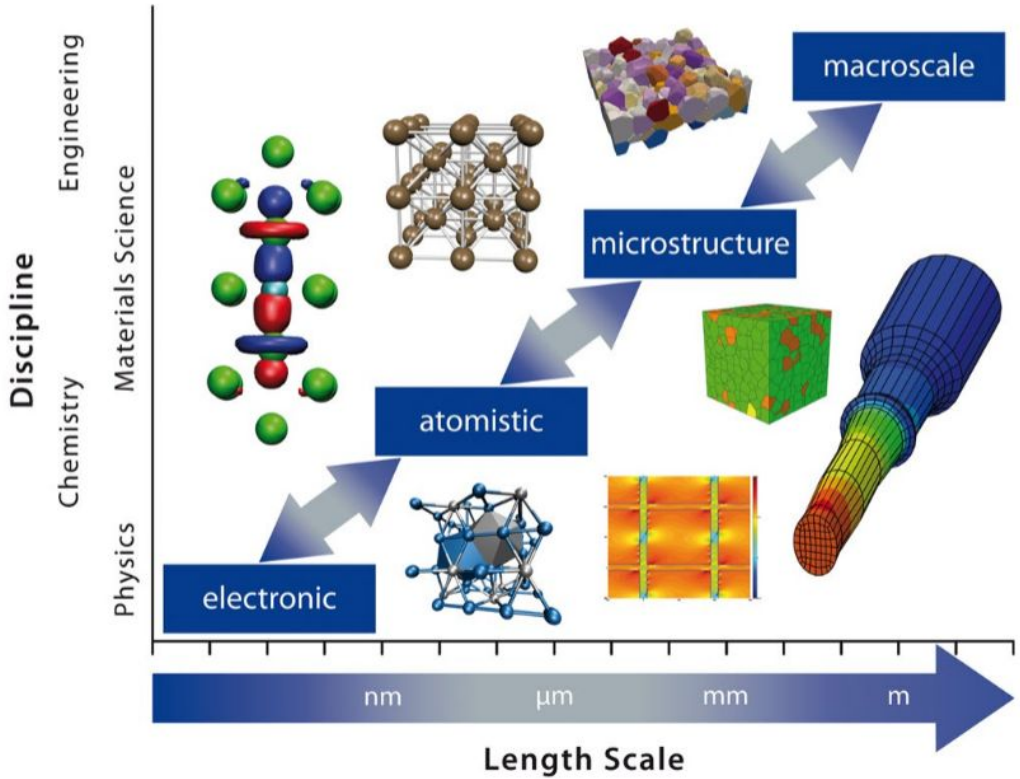
Conveners: Paul Romano (ANL), Paul Wilson (UW-Madison)

Workshop for Applied Nuclear Data Activities (WANDA) 2024
February 27, 2024

Speakers

- Guinevere Shaw: Office of Science/Fusion Energy Sciences
  - FES perspectives on material damage
- Mark Gilbert: UKAEA
  - Nuclear data applications to integrated modeling of materials damage
- Dieter Leichtle: KIT
  - Status of complete neutron-induced displacement damage cross-section data
- Lee Bernstein: UC-Berkeley/LBNL
  - Fast neutron irradiation of high temperature superconducting materials
- Hesham Khater: LLNL
  - Radiation damage to electronics at NIF
- Shengli Chen: Sun Yat-sen University (presented by P. Romano)
  - Efforts to improve the accuracy of calculated displacement damage

Integrating Across Length Scales



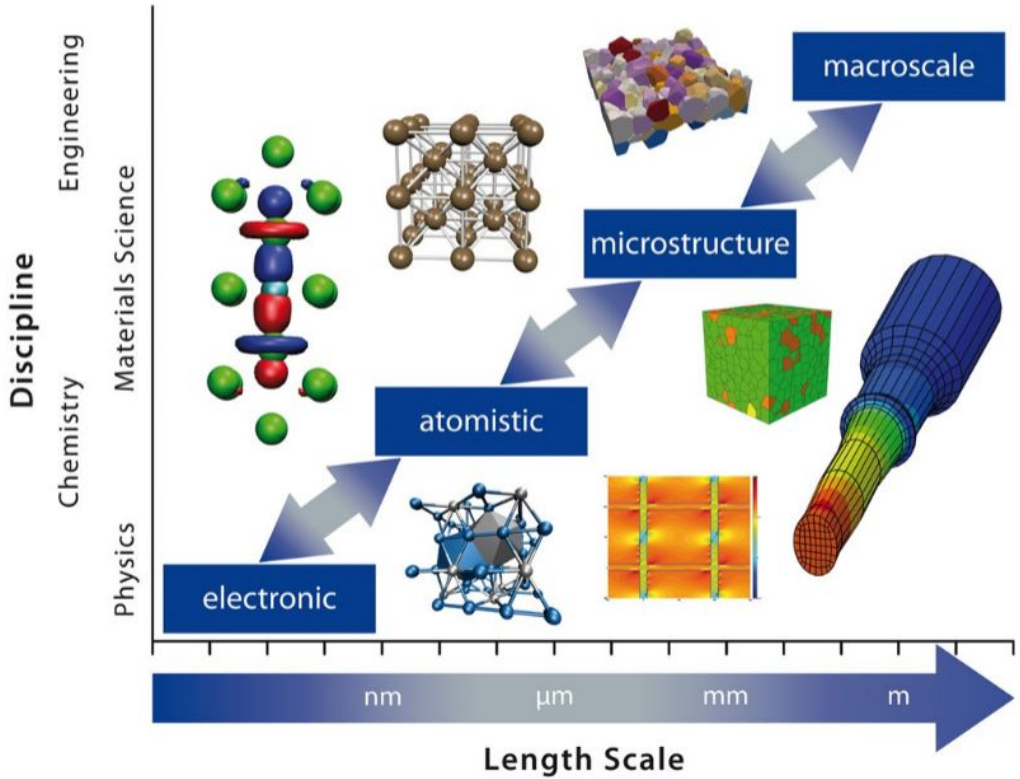
Material damage cross-sections define the consequences of individual interactions at the atomistic scale

Variety of responses of interest

- atomic displacements*
- gas generation
- transmutations

*Limited ability to directly measure atomic displacements

Integrating Across Length Scales



Engineering scale material performance is a non-linear consequence of accumulated atomistic events and the environmental history

Different combination of different atomistic events result in different performance

Unlike many other engineering responses

Limited ability to simulate across length scales

Why Not Use Already Qualified Materials?

- No structural materials have been qualified at end-of-life conditions for fusion structural materials
  - Especially combination of DPA and He gas production (10 appm/DPA)
- Structural materials dominate radioactive material generation
  - Seek novel reduced activation alloys to minimize operation dose rates and waste disposal inventories
- Impact of material choices on tritium breeding and shielding performance
  - See session III
- **What about other materials? Diagnostics, electronics, magnets, etc?**

Atomic Displacements (DPA)

- Integral dose measure
  - Used to correlate the irradiation environment experienced by an experimental specimens with the irradiation environment expected in a future energy system to predict bulk material performance
- Alternative models exist for estimating DPA (Leichtle, Chen)
  - Difference depends on assumptions of recombination of Frenkel pairs following initial displacements
  - May result in different spread/clustering of irradiation environment assessments
- Models sensitive to input parameters
  - Especially assumed value of energy required to produce each Frenkel pair (Leichtle, Chen)
- All models relies on PKA recoil spectrum as primary input
  - Key opportunity for improved nuclear data
  - Some specific evaluations have been shown to have questionable recoil data (Chen)
  - Charged particle production spectra also important

Atomic Displacements (cont'd)

- PKA recoils produce cascades of displaced atoms (Gilbert)
  - Direct modeling of these cascades can result in understanding of microstructure changes
  - Long way to go to translate this to bulk material performance (with no(?) additional nuclear data needs)

- SPECT-PKA generates PKA distributions for use in atomistic scale simulation

Non-Structural Materials

- Novel high-temperature superconductors: REBCO/BSSCO (Bernstein)
  - Thick-target deuteron breakup (TTDB) neutron flux spectrum, d + Be, at LBNL 88-inch cyclotron (0.3 milli-IFMIF)
  - Useful environment for gas production & transmutation measurements
  - Collaboration to determine impact on superconductivity

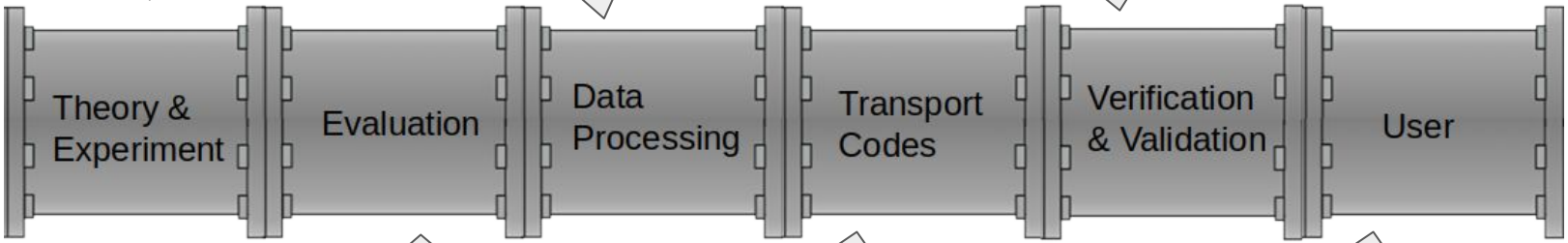
- Variable performance of electronics at NIF under irradiation (Khater)
  - Need environment to characterize performance across commodity components

Discussion questions as they relate to the “pipeline”

- How good are our cross sections?
- Do we have sufficient measurements of cross sections relevant to DPA?
- What nuclides/reactions need more focus?

- What improvements are needed in damage models?
- How else can we improve our data processing codes to produce robust DPA cross sections?

- How should validation of DPA be performed?
- What experimental capabilities are needed?
- Are our V&V processes adequate for catching problems with DPA?



- What improvements are needed in evaluations or the evaluation processes?

- What improvements are needed in transport codes to better assess DPA?

- How can we relate simulation to reality (change in material properties)?
- What does materials community view as important for us to provide?

Discussion - Nuclear Data Needs

- Lack of prioritization from fusion community
  - Sensitivity studies needed to identify most important nuclear data
  - Experiment similarity assessment to ensure new measurements are relevant, esp. integral benchmarks
  - Prioritization between damage-relevant data and other priorities (e.g. data relevant for tritium breeding - see sessions II & III)
- Improved recoil/charged particle spectra will facilitate better DPA estimates
  - Better ultimate correlation between irradiated bulk samples and predicted power plant environments
  - Unclear whether multi-scale computational assessment will be robust enough for predictive material performance
  - Still needs novel intense source (FPNS/IFMIF) for testing bulk materials at realistic irradiation conditions

Discussion - Leveraging Existing Facilities

- Performance of non-structural materials in fusion-relevant spectrum
  - Magnets, electronics, diagnostics, windows, etc
  - Fundamental nuclear data needs unclear
  - Little database for basic assessment of radiation effects

- Activation data improvements can be achieved at existing facilities
  - Important threshold reaction channels may be less-well characterized in lower energy systems
  - Also may need improved branching ratio information, esp. w.r.t. isomeric states
  - This may be a valuable near term benefit for systems being built prior to pilot plants

Other Discussion

- Improved recoil data in some evaluations in ENDF/B-VIII.1
- Little evidence of important cross-section temperature effects on typical fusion nuclear responses
- Confirm role of temperature dependence
  - Important for other physics, e.g. annealing
  - Appears less important for direct nuclear data responses

Recommendations

- Review consistency of recoil data across evaluations
- Update processing tools to support wider variety of DPA models
- More comprehensive sensitivity analysis to determine most important nuclear data across different integrated design models
  - Most urgent may be support for licensing and operation of pre-pilot plant facilities
    - Activation data to support licensing
    - Predicting performance of electronics, diagnostics, etc, to support operation
  - Prioritize experimental measurements, both differential and integral