

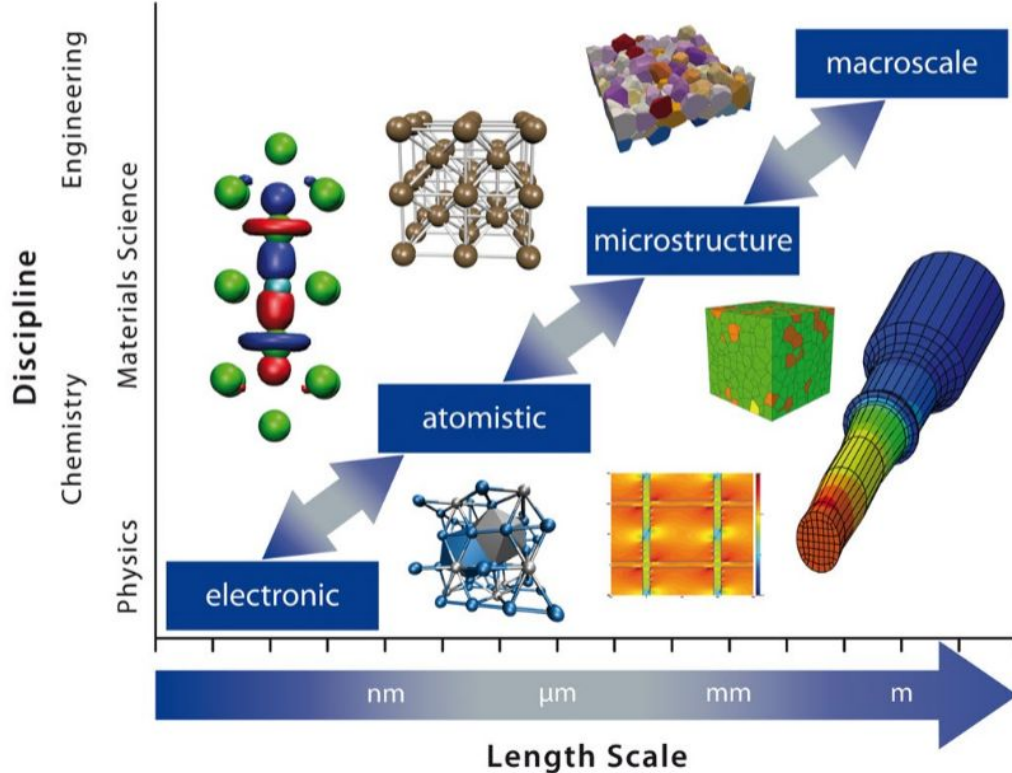
Session IV: FES Materials Damage

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Workshop for Applied Nuclear Data Activities (WANDA) 2024
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Theoretical Background

Integrating Across Length Scales



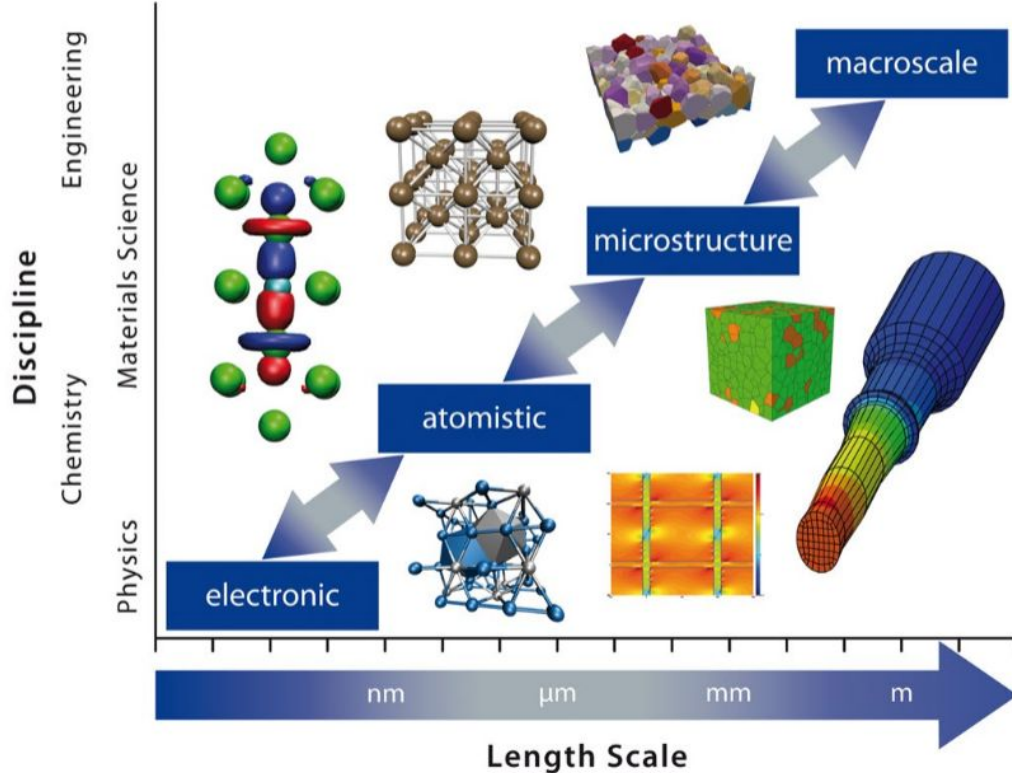
Material damage cross-sections define the consequences of individual interactions at the atomistic scale

Variety of responses of interest

- atomic displacements*
- gas generation
- transmutations

*Limited ability to 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 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 reduced activation alloys to minimize operation dose rates and waste disposal inventories
- Impact of material choices on tritium breeding and shielding performance

Displacement cross section

$$\sigma_D(E_n) = \sum_j c_j \sum_i \sigma_{i,j}(E_n) \int f_{i,j}(E_n, \mathbf{X}) E_D(E_R(E_n, \mathbf{X})) d\mathbf{X}$$

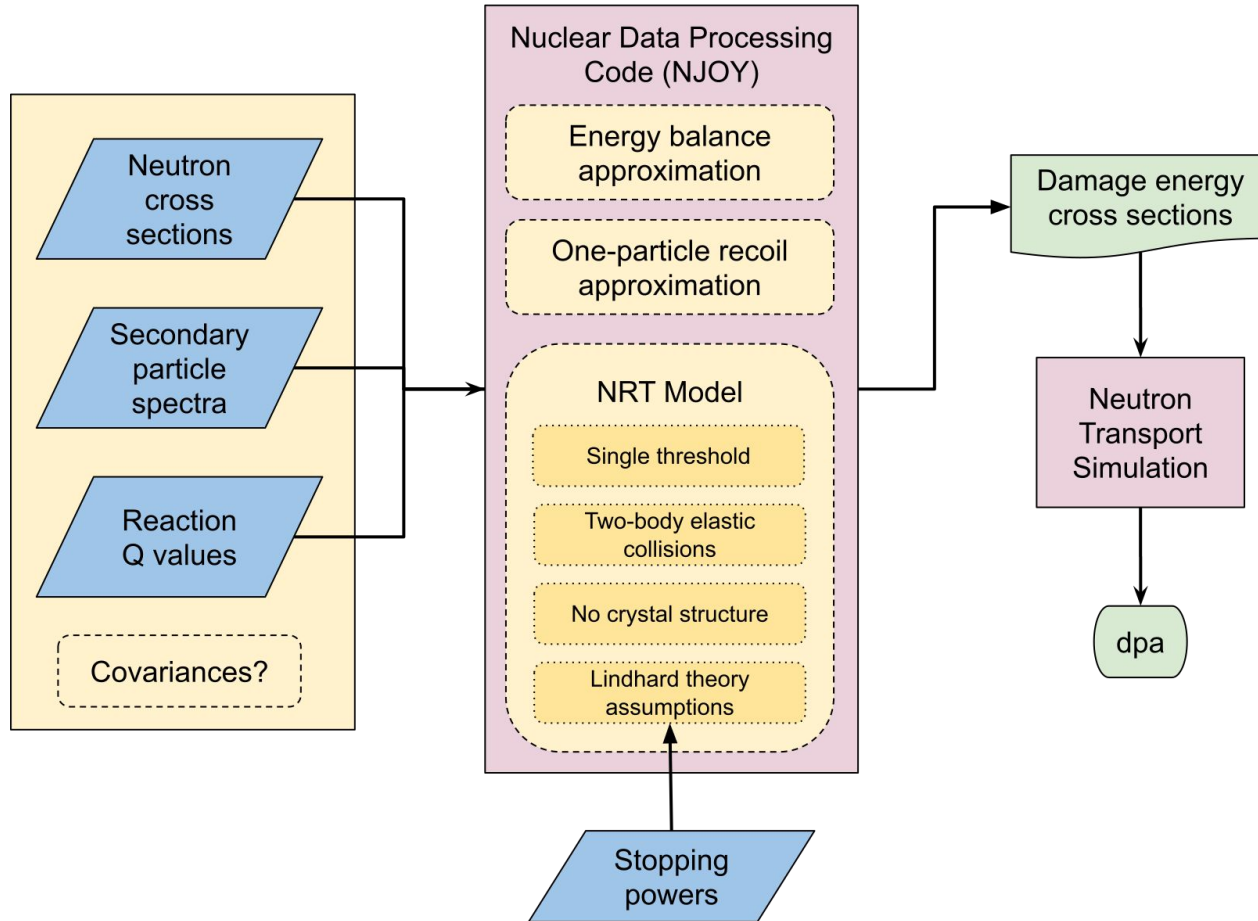
Cross sections

Recoil distribution

Damage model

The diagram shows the equation for the displacement cross section, $\sigma_D(E_n) = \sum_j c_j \sum_i \sigma_{i,j}(E_n) \int f_{i,j}(E_n, \mathbf{X}) E_D(E_R(E_n, \mathbf{X})) d\mathbf{X}$. Annotations include: 'Cross sections' pointing to the $\sigma_{i,j}(E_n)$ term; 'Recoil distribution' pointing to the $f_{i,j}(E_n, \mathbf{X})$ and $E_R(E_n, \mathbf{X})$ terms; and 'Damage model' pointing to the $E_D(E_R(E_n, \mathbf{X}))$ term. The terms are highlighted with colored boxes: $\sigma_{i,j}(E_n)$ is green, $f_{i,j}(E_n, \mathbf{X})$ is blue, $E_D(E_R(E_n, \mathbf{X}))$ is pink, and $E_R(E_n, \mathbf{X})$ is also blue.

How we get from nuclear data to dpa



WANDA 2019 Summary

WANDA 2019 Findings/Recommendations

- ENDF is missing data for recoils and (n,α)
 - Inaccurate (n,α) data caused serious miscalculation of material lifetime
- Need to understand how changes in material properties affect neutronics
 - Transmutation, porosity, chemical bonds
- Processing of data in NJOY needs modernization to meet the needs of the fusion community
- Current models do not determine the size of vacancies
- Stopping powers are not well understood
- Radionuclides produced under transmutation might create further PKAs as they decay and must be quantified
- Inelastic scattering cross sections need to be improved for fast energies
- Secondary particle production is not well known and requires measurement and theory development

WANDA 2019 Findings/Recommendations

There should be a coordinated and comprehensive materials damage database for validation of calculations

- INL has a database of irradiated materials (irradiation data but no post-irradiation testing data)
- Improved dosimetry standards will be necessary for 14 MeV neutrons
- Post irradiation testing
 - Several capable laboratories with full suite of testing
- Need to standardize materials analysis methods and format for irradiated materials data

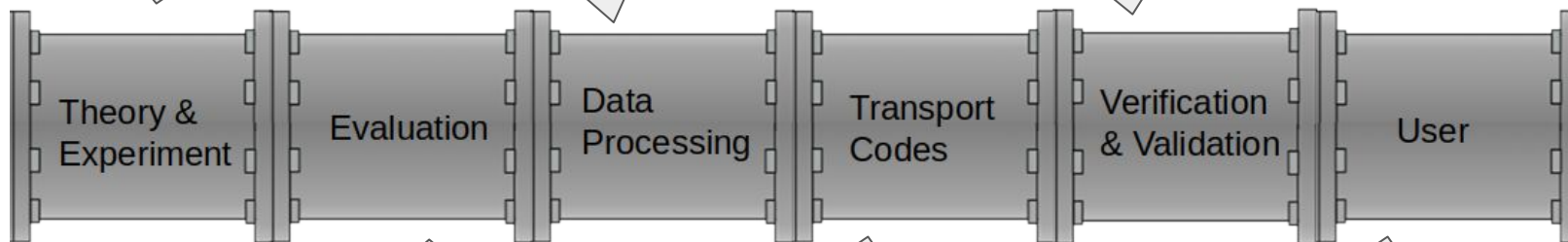
Questions for Discussion

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?