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Notes for the closing discussion

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Core questions for plasma-material interaction in fusion devices

Studies of PMI in fusion devices have two main concerns:

- Erosion
  - Lifetime of plasma-facing components
  - Damage (cracking, blistering)
  - Impurity production
- Hydrogen (tritium) retention
  - Deposition (penetration, codeposition)
  - Retention (trapping)
  - Migration

Relevant interests in radiation damage:

- Characterize microstructure after irradiation (defects, H+He clusters)
- Study the influence of microstructure on properties of tritium retention
- (Also structural properties: embrittlement, D/B transition)

Tungsten is of highest interest, then steels, and note role of liquid metals, beryllium and graphite/CFC in fusion research. Note mixed materials and alloys.

Core questions for PMI …

Slightly more focussed:

- Erosion
  - Characterize differential erosion of RAFM steel; self-passivating behaviour?
- Hydrogen (tritium) retention
  - Characterize effect of defects on tritium transport in W
  - Characterize mutual effects of H and He in W
- Radiation damage
  - How can ion beams be used to approximate neutron damage?
- Experiment
  - Can we simulate time-programmed thermal desorption spectroscopy?

Basic tools:

- Electronic structure theory (in practice, DFT)
- Fitted Potential Energy Surface (PES) or Force Field (FF)
- Molecular Dynamics (MD) simulations
- Kinetic Monte Carlo (KMC) simulations

Sources of uncertainty

Standard approach via ES/DFT + PES/FF + MD + KMC:

- Fundamental
  - Non-BO effects, electronic excitation (think of PKA events in radiation damage; material ablation under pulsed loads)
- Uncertainties in ES/DFT calculations
  - Really it is the Density Functional Heuristic; no systematic path for improving the functional
  - Practical difficulties for amorphous material, complex alloys, real steel, liquid state; anything that needs a large unit cell
- Uncertainties in the fitted PES/FF
  - Domain of accuracy; is it adequate for energetic events?
  - Accuracy for basic energy landscape, adequate for all relevant TST?
- … (Continued next slide)

For discussion: What is the relative importance of the above uncertainties?

More pointed: Which is worst, the DFT or the PES?

Sources of uncertainty, …

Standard approach via ES/DFT + PES/FF + MD + KMC:

- Molecular Dynamics (MD) simulations
  - Quantum effects on nuclear motion (e.g. H transport at low temperature)
  - Artificial enhanced source term, artificial timescale, but diffusion is not enhanced
- Uncertainties in Kinetic Monte Carlo (KMC) simulations
  - Rates obtained from ES/DFT energies and Arrhenius theory; is it adequate?
  - Problems with complex landscape, many transition paths; do we have a correct inventory?

For discussion: What is the relative importance of the above uncertainties?

For MD at highly enhanced source rate, do we need to use a PES that is fitted to similarly enhanced kinetics rather than to real (ES/DFT) energetics?

Experiment to the rescue?

Interpretation of experiments

Key quantities from experiment, if they could be provided:

- Microstructure, defect types, defect concentration
  - Atomic force microscopy?
  - Positron annihilation spectroscopy?
  - Thermal desorption spectroscopy?
- Concentration profiles of H and He in the near-surface layer and bulk
  - Ion beam analysis?
  - Nuclear reaction analysis?
  - Real-time exposure, supersaturation?

For discussion:

- What can the modellers do more to support interpretation of experimental data?
- Is there particular data that modellers can ask of the experimentalists?
- One specific diagnostic, (time programmed) thermal desorption spectroscopy. Are we doing the best job in interpreting those data?