Why is IFMIF crucial for enabling predictive modelling of material degradation in fusion power plants?

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Damage on materials from fusion plasmas

- There are two main types of damage on materials in fusion reactors:

  1. Surface damage from hot nuclei hitting the inner walls (plasma-material interactions)

  2. Damage on materials everywhere from the ~14 MeV neutrons produced in the fusion reaction
Nature of neutron damage

- The neutron cross-section is low, so they travel deep.
- However, with some cross-section they collide with a nucleus and give it a high recoil energy (keV’s to 100’s of keV’s).

Damage event by 10 keV Fe recoil in Fe

[K. Nordlund et al, Nature communications 9, 1084 (2018)]
Motivation: Radiation damage in nuclear reactors

- Via a complex set of additional this nanoscale damage eventually leads to major macroscopic consequences: changes of mechanical properties of materials, swelling, embrittlement, …

Test samples put for many years in a fission reactor


What happens physically in the materials during the continued neutron irradiation?

- **Length**
  - m (meter)
  - mm (millimeter)
  - μm (micrometer)
  - nm (nanometer)

- **Time**
  - ps (picosecond)
  - ns (nanosecond)
  - μs (microsecond)
  - ms (millisecond)
  - s (second)
  - hours
  - years

**Events:***
- **Primary damage production (cascades)**
- **Bubble formation;**
- **Defect and implanted ion mobility, recombinations**
- **Dislocation mobility and reactions**
- **Swelling**
- **Changes of macroscopic mechanical properties**
What is used to model all this: the materials multiscale modelling framework

- Sequential and concurrent multiscale modelling
- In Europe EUROFUSION WPMAT IREMEV has great coordination

![Diagram showing various scales and models](image-url)
Need for IFMIF, part 1

- The general picture is known, as are methods needed to model it. Fission reactors have been used to study bulk neutron damage for years
- **WHY IS IFMIF then needed??**
- The obvious answer: Fission reactors have a very different neutron spectrum than fusion ones. In fission ~1 – 5 MeV neutrons dominate damage, while in fusion there is a huge 14 MeV neutron flux
- There is no high-efficiency 14 MeV fusion source in the world
- However, one could ask: why not just count the damage as:
  - 14 MeV neutron damage = 4 x (3.5 MeV neutron damage) ??

[M. Gilbert et al, 2013]
Need for IFMIF, part 2

- Although we do not have a high-efficiency 14 meV neutron source yet, we do know that:
  - 14 MeV neutron damage ≠ 4 x (3.5 MeV neutron damage) !!

- There are two main reasons to this:
  1. The nuclear reactions for > 10 MeV neutrons are much more complex than those for few MeV ones
     - In the low-energy case, damage is dominated by simple elastic nuclear collisions, for which recoil spectrum is well known
     - 14 MeV neutrons also produce lots of inelastic nuclear reactions that e.g. lead to He production and nuclear transmutations
  2. Even the damage produced by the simple elastic collisions is qualitatively different for 14 MeV neutrons
Motivation of part 1: Neutron-induced transmutations

- Video from Mark Gilbert on neutron-induced transmutations in W over 5 years of DEMO operation
- Shows a major materials physics challenge: material does not stay the same!
- Note also H, He production
Motivation of part 2: damage by fusion neutrons

- Roughly speaking: typical fission neutron recoil E is about 10 keV in W, typical fusion neutron about 150 keV
- The higher energy can produce huge damage clusters immediately
  => qualitative difference between fission and fusion!
Why does the damage clustering matter?

- There is clear simulation evidence that the long-term damage evolution is dominated not by point defects, but by large clusters.
- This is (unfortunately) also where the simulation model reliability limit comes in: different interatomic potentials predict different fractions of damage in large clusters.

Need for IFMIF, part 3

- There are of course efforts to make the simulations more reliable, and to validate the models with non-neutron experiments
  - Ion beam experiments can to some extent model the neutron damage, and are very useful for simulation validation
- However, the complexity of the processes going on is enormous, and there are major unknowns along the way
- There are known unknowns, and probably also unknown unknowns
Complexity of processes

- All of the following are known to happen. However, many of these processes cannot be simulated predictively alone, and the concerted actions certainly not.

This schematic is intentionally messy – since so is reality
Conclusion

- The damage buildup processes are very complex, and understanding of them is mainly at a qualitative level so far
  - Reaching predictive modelling over all scales is not impossible, but will need huge efforts and decades of time

- To be able to do reliable materials selection for DEMO and design it on schedule, we really need IFMIF/DONES now!
Backup slides
New models to make formulation of higher-scale models easier

- Most recently, we developed new analytical models to describe the damage behavior in a simple consistent manner.
- Instead of using millions of CPU hours one can get the results with a simple analytical equation:

\[ N_d(E) = \begin{cases} 
0 & E < E_d \\
1 & E_d < E < 2E_d / 0.8 \\
\frac{0.8 E}{2E_d} \xi(E) & 2E_d / 0.8 < E < \infty 
\end{cases} \]

\[ \xi(E) = \frac{1-c}{(2E_d/0.8)^b} E^b + c \]

[K. Nordlund et al, Nature communications 9, 1084 (2018)]
Highlights of results 2015

1. Including carbides in DDD simulations

- In an Academy of Finland nuclear technology project joint with Mikko Alava (Aalto) we are using MD to parametrize DDD on dislocation-impurity precipitate interactions
- Example: Fe edge dislocation – cementite precipitate

[Lehtinen, Granberg, Laurson, Nordlund, Alava, submittedish (2015)]
2. New dpa equation with realistic description of damage – outcome of OECD NEA group

The traditional “dpa” equation for estimating neutron and ion damage is well known to be about a factor of 3 wrong.

Within an OECD NEA group we devised an improved form:

$$N_d(E) = \begin{cases} 
0 & E < E_d \\
1 & E_d < E < 2E_d / 0.8 \\
\frac{0.8E}{2E_d} \xi(E) & 2E_d / 0.8 < E < \infty
\end{cases}$$

where the new term $\xi(E)$ is given by

$$\xi(E) = \frac{1-c}{(2E_d/0.8)^b} E^b + c$$

[Nordlund et al, OECD NEA PRD group final report, OECD (2015)]
Highlights of results 2015

2. New dpa equation with realistic description of damage – outcome of OECD NEA group

- This form gives very good fit to composite MD and experimental data

\[ \xi = 0.201 \exp^{-0.628} + 0.283 \]

\[ \xi = (1 - 0.286/(2E_d/0.8)^{-0.568}) \exp^{-0.568} + 0.286 \]
Highlights of results 2015

3. Systematic collection of data for ERO calculations [FZJ collaboration]

- We are simulating the D bombardment of Be reflection and sputtering yields as a function of wall T, energy and D concentration for ERO multiscale modelling
  - Huge differences in D behavior as a function of Be
In a close collaboration with CCFE we showed that MD simulations can obtain outstanding agreement with experiments on cluster size distributions.

- First time ever cluster size distributions in metals measured over a wide size range!