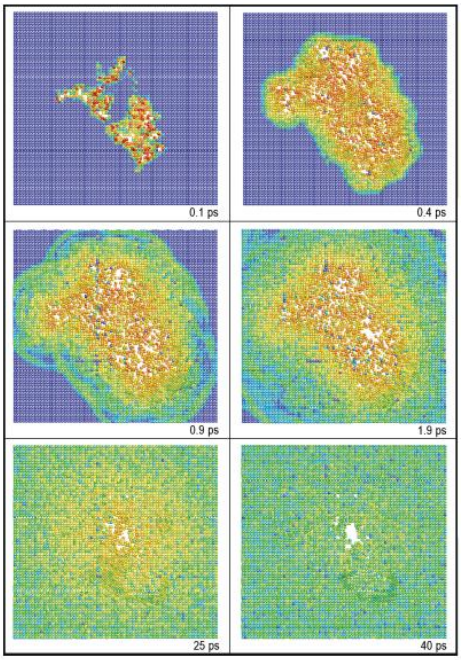
Project 1: Predictions of primary radiation damage with two-temperature molecular dynamics



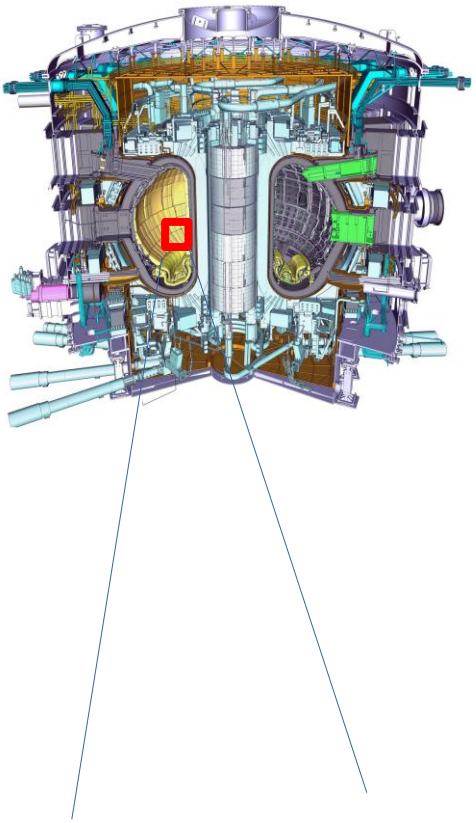
The damage in materials created by energetic impacting particles is highly sensitive to the mechanisms of dissipation of the impinging particle's kinetic energy. This summer project involves performing two-temperature molecular dynamics (TTMD) simulations of collision cascades (see image), employing a recently developed model, which accounts for electronic energy dissipation in unprecedented detail [1], to predict the primary radiation damage under different incident ion energies. While the TTMD method accounts for the thermal conductivity of the electronic system through a heat diffusion equation, the possible effects of atomic disorder in reducing the local electronic conductivity have not to date been investigated.

In this project, the effects of electronic thermal conductivity will be investigated by varying the implementation of the electronic system grid. Focus will be on analysis of the surviving damage, including defect numbers and defect morphology. The student will gain knowledge of the processes of radiation damage formation in materials, learn the basics of performing molecular dynamics simulations of highly non-equilibrium events, and develop a familiarity with high performance computing environments. Depending on the skills and interests of the student, code development can also be a part of the work. This project is suitable as a basis for either a MSc or BSc thesis.

Necessary skills: Experience in programming or scripting, e.g. with Python, is highly desirable. The candidate should also have basic knowledge of solid state physics.

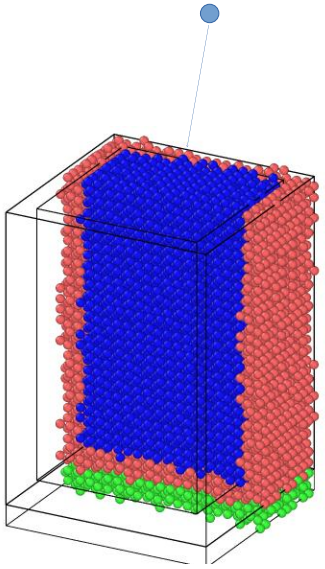
[1] Tamm, A., *et al.*, Phys. Rev. Lett. **120**, 185501 (2018)

Project 2: Surface material erosion in nuclear fusion devices



Understanding plasma-wall interactions is one of the main challenges in the design and development of fusion reactors. Among the primary effects of these interactions is the erosion of plasma-facing components through physical or chemical sputtering, which can limit the availability and performance of the device.

The work in this project involves performing molecular dynamics simulations of low-energy plasma particle impacts on materials used for plasma-facing surfaces. Results can be used for predictive modelling of surface erosion, plasma contamination, in plasma transport codes, etc. …



Some of the factors of interest include:

- the effect of surface orientation and surface morphology on the above quantities
- details of ion-electron interaction (electronic stopping) and the impact of this on predictions
- fidelity of interatomic potentials (in particular short range interactions)

Necessary skills:

- Familiarity with the Linux operating system and with Python
- basic knowledge of solid state physics
- basics of performing molecular dynamics simulations of non-equilibrium events
- familiarity with high performance computing environments