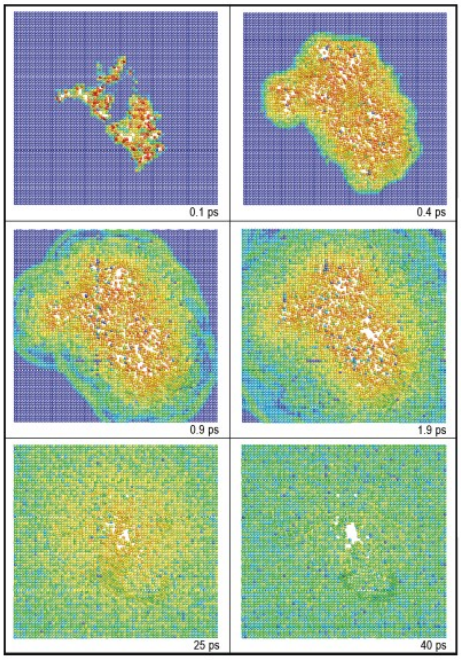
Project 1: Effects of electronic conductivity on damage formation and defect morphology in metals



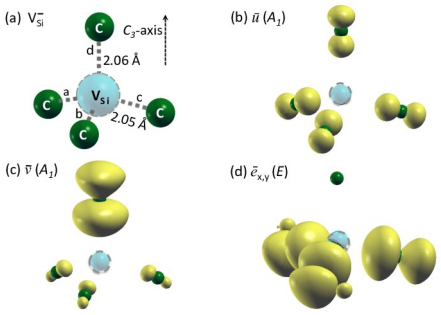
The damage in materials created by energetic impacting particles is highly sensitive to the mechanisms of dissipation of the impinging particle's kinetic energy. This summer project involves performing two-temperature molecular dynamics (TTMD) simulations of collision cascades (see image), employing 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: Electronic structure calculations of radiation-induced defects in semiconductors



Electronic structure

Ion implantation is used widely for material modification, particularly in the semiconductor industry. In addition, many semiconductor devices are employed in high radiation environments. However, ion irradiation creates lattice defects, which degrade the electronic properties of semiconductor materials. In this project, the student will carry out first principles calculations of the electronic structure of defects formed dynamically in large scale atomistic simulations of radiation damage in semiconductors. The electronic structure of the defects ultimately is responsible for leakage or breakdown in electronic components, hence predicting the radiation hardness of components requires knowledge of the electronic states of the radiation-induced defects.

Necessary skills: The candidate should have basic knowledge of solid state physics, and computational methods in physics or material science. Familiarity with the Linux operating system is essential. Experience with bash scripting and/or python is considered a merit.