Atomic scale modelling of radiation damage

PhD scholarship

The effect of radiation on materials has important consequences to many fields, from solar cells to satellites, from radiopharmaceuticals to fusion energy, from engineering non-destructive testing to fission reactors. When radiation interacts with the materials, individual atoms may be knocked off their crystal lattice, and leave behind defects. This process is known as *radiation damage*, and may lead to changes in the material's physical, chemical and mechanical properties, known as *radiation effects*.

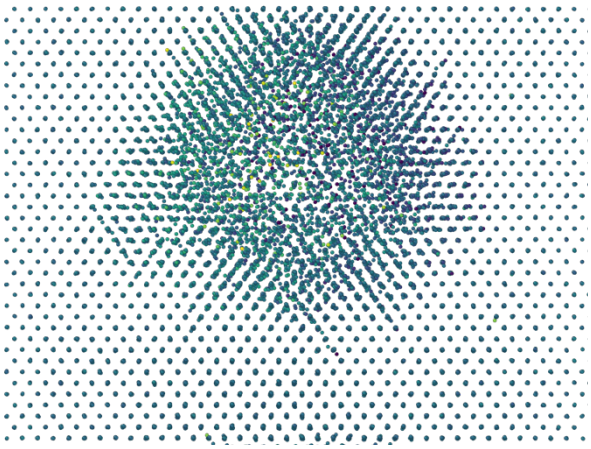

Figure 1 – Example of atomic scale simulations of radiation damage. This is a snapshot of a collision cascade in a metal

Whether the radiation effects are detrimental, tolerable, or even beneficial depends entirely on how the defects evolve after they have been created: do they annihilate with one-another, or do they cluster into larger defects? are the defects mobile or sessile? Can they be annealed by heating or by deformation? Understanding the radiation damage process, and the subsequent evolution of the damage created, is an essential step in the design of novel materials that are either more resistant or more tolerant to radiation. Atomic-scale simulations are an invaluable tool to shed light on the complex interaction between defects, and predict how different materials will respond to different radiation environments.

In this project the student will perform atomic scale simulations of radiation damage in advanced materials, and will contribute to the development of new simulation methods for modelling of defect in materials. This will include new force fields for molecular dynamics (possibly through machine learning techniques), and the accelerated methods to describe concentrated defects in solids.

The candidate will be based at UNSW Sydney, in the AtomCraft research group led by Dr. Patrick Burr. We are a tight-knit, inclusive, and enthusiastic group of diverse background. We value diversity and encourage applications from all backgrounds to apply. A background in materials science/engineering or solid state physics is beneficial, as is competence in computer languages and programs.

The project is supported by a generous scholarship of $38,600/year stipend plus $10,000 of travel support, provided by a philanthropic donor. Candidates with an exceptional track record may be eligible for additional scholarship top-ups. Send email applications and queries to p.burr@unsw.edu.au. When applying, please include your CV and transcript of most recent or current degree.