Modelling of radiation damage in diamond

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Funding: Fully funded PhD studentship (48 months).
Start date: September/October 2023.
Application deadline: Ongoing

The modelling of radiation damage in diamond and other crystalline materials is inherently a multi-scale problem with a range of processes occurring over multiple different length (e.g., atomic to mm) and time scales (e.g., < fs to >10^3 s). Irradiation with energetic photons, electrons, or ions creates significant primary electronic excitation and secondary electrons or photons (fs timescale). If sufficient energy is transferred to an atom, this can be displaced from its lattice site creating a vacancy. The displaced atom can recombine with the vacancy, come to rest as an interstitial defect, form a complex with another defect or if it has sufficient energy, it can go on to displace further atoms. The electronic excitation leads to the formation of free carriers, excitons or at high excitation densities an electron-hole plasma. The energy delivered to the electronic system is exchanged with the atomic lattice (typically ps-ns time scales) and can result in heating, and even phase transitions (e.g., conversion of diamond to graphite).

If mobile, the vacancies and interstitial atoms produced can interact with each other and pre-existing defects and impurities in the diamond to produce a vast array of complexes, some of which may only be metastable and in turn be converted into more stable defects. Important processes, such as diffusion are often controlled by defects, and the clustering of point defects can lead to the formation of extended defects such as dislocations. These complicated, both short- and long-range processes, defect interactions and transport must be considered and their evolution under irradiation is a highly stochastic process which depends, among other aspects, on the initial spatial arrangements of impurities and dislocations, and of course close to surfaces outcomes can be very different to those in the bulk.

Ab initio quantum-mechanics based methods (e.g., DFT - Density Functional Theory) can provide information about the structures of point defects and the nature of their interactions at short range (atomic distances). Molecular dynamics (MD) simulation is a method where the trajectories of atoms are determined by numerically solving Newton's equations of motion, where forces between the particles and their potential energies are calculated using empirical interatomic potentials. MD has been widely used to study radiation damage in materials using the primary knock-on atom method, to provide an atomic level description of the complex defect morphology resulting from the impact of a high energy particle. The predictive ability of classical MD simulations depends on the reliability of the empirical potential model used to describe the interactions between the atoms in the crystal. Recent developments in machine-learned potentials means that ab initio accuracy can be routinely achieved in MD calculation at a very low computational cost. Mesoscale methods go beyond the atomistic models, to simulate defect evolution at much longer time scales. For example, object kinetic Monte Carlo (OKMC) is a computational method able to extend the time and length scale of molecular dynamics simulations to times and sizes that are comparable to experimental observations. OKMC calculations obtain input from for example, DFT and MD simulations, in order to have reasonable physical inputs for the migration and attempt frequencies of all the objects (e.g., point defects, clusters, dislocations, etc) that can form, their interaction volume, and the dissociation energies of all

the possible objects that can be emitted. Selection of the processes that should be included, and the physical inputs determining the probabilities of different events are at the discretion of the modeler, so comparison with experimental data, where outcomes are known, is essential to build faith in the predictive capability of this approach.

In this project the PhD student will utilise the outputs of atomistic modelling and experimental studies to develop mesoscale modelling methods such as OKMC to simulate radiation damage defect production and evolution in diamond. Although a modelling project, it is essential that student works closely with experimentalists, to understand the input data produced by a wide range of different irradiation and annealing experiments. The goal is to develop a modelling package that can be used predictively to determine the outcomes of irradiation of intrinsic and doped diamond with energetic photons, electrons, or ions. Experimentally both the doping concentrations (for impurities such as nitrogen and boron) and irradiation doses can be varied by over six orders of magnitude, and of course in addition to point defects diamond can contain significant densities of dislocations. This wide variation provides a robust check for the validity of the model. There is considerable interest in irradiation of diamond, examples include the efficient production of nitrogen-vacancy defects without residual damage for a range of quantum technologies, understanding how diamond detectors operate under extraordinary radiation damage fluxes in fusion reactors or the next generation of particle accelerators, or even how evaluating diamond devices for space-based missions.

Applicants should have an honours degree (at least 2.i or equivalent) in physics, chemistry, or materials science. A strong interest in materials modelling using ab initio and machine learning methods is essential. Experience with computing tools, such as Python and atomistic modelling software would be beneficial.

The student will join a team of over 40 researchers in the diamond community at Warwick (academic research groups spread in Warwick Chemistry, Physics and Engineering) and benefit from a wide range of interactions. The studentship will commence in October 2023 (although an earlier start is possible based on your availability) and will provide a maintenance grant and tuition fees at the standard UK rate, currently set at £18,200 for the 2023/24 academic year. Funding may be available on a competitive basis to exceptional students of any citizenship. Applications are welcome to those able to support themselves or with funding already arranged. Such applications will go through the same level of academic assessment.

For further details please contact, Dr Albert Bartok-Partay (Albert.Bartok-Partay@warwick.ac.uk), Dr Ben Green (b.green@warwick.ac.uk), Prof Mark Newton (m.e.newton@warwick.ac.uk) and DST.Admin@warwick.ac.uk, along with a CV.