Application for a TSM-DTC funded PhD studentship

Please complete this form electronically
and submit to Lilian Wanjohi (l.wanjohi@imperial.ac.uk)
by Friday January 8, 2010

1st supervisor
Name: Matthew Foulkes
CID (IC only): 00007151
Institution, Department, Address: Imperial College, Physics, South Kensington Campus
Email: wmc.foulkes@imperial.ac.uk
Phone: 020 7594 7607

2nd supervisor
Name: Andrew Horsfield
CID (IC only): 00523934
Institution, Department, Address: Imperial College, Materials, South Kensington Campus
Email: a.horsfield@imperial.ac.uk
Phone: 020 7594 6753

3rd supervisor (optional)
Name: Dan Mason
CID (IC only):
Institution, Department, Address: Imperial College, Physics, South Kensington Campus
Email: d.mason@imperial.ac.uk
Phone: 020 7594 7542

Please complete the following:

1. Project title

What excited electrons do.

2. Project abstract (≤ 200 words please and please add 1 or 2 key references)

While often treated as such, electrons are not Stepford Wives that slavishly follow their nuclei (the Born-Oppenheimer approximation). Indeed their excited states contribute to many important properties of materials such as electrical conductivity, thermal conductivity, colour and reflectivity. For several years we have been investigating the contribution of electronic excitations to the radiation damage created in metals by high energy neutrons (J. le Page, D.R. Mason, C.P. Race and W.M.C. Foulkes 2009, "How good is damped molecular dynamics as a method to simulate radiation damage in metals?", New J. Phys. 11, 013004). This work has primarily involved atomic scale simulations, but we would now like to extend it to longer length and time scales by introducing suitable mesoscopic models. We have begun this process, but there is still far to go. We would also like to go beyond metals to include insulators as radiation damage in these materials is very important (for example, see Jiang W et al. 2009, "Response of Nanocrystalline 3C Silicon Carbide to Heavy-Ion

Irradiation." Physical Review. B, Condensed Matter 80, 161301). The study of insulators introduces new challenges as we now have to consider excitons (bound electron-hole pairs that can either be mobile or trapped). We have experience of modelling excitons trapped by the displacement of atoms, and will bring this to bear on this project. Once excitons are formed, they can hop stochastically, a process we will model using kinetic Monte Carlo.

3. What is the multi-scale nature of the project? (≤ 100 words please)

Atomistic and electronic data will be obtained using tight binding as implemented in the code spICED. Longer length scale simulations of the relaxation of electronic excitations in metals will be performed using the diffusion equation for heat transport, with local structure- and damage-dependent diffusivities obtained from the tight-binding simulations. For insulators, kinetic Monte Carlo simulations of exciton hopping, and its impact on the atomic structure, will enable us to reach greater length scales in insulators.

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)

Matthew Foulkes: electron correlation
Andrew Horsfield: Monte Carlo with electrons; empirical Hartree-Fock.
Dan Mason: spICED

5. Is there a self-contained 12-week MSc project that would usefully initiate this PhD project? (If the answer is no the project will not be offered as an MSc project)

spICED simulations with an sp3 tight binding model of silicon to obtain some initial insights into the influence of bandgaps on radiation damage.