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: Mark Wenman
CID (IC only): 600593
Institution, Department, Address: Imperial College London, Department of Materials
Email:m.wenman@imperial.ac.uk
Phone:0207 594 6763

2nd supervisor
Name: Alessandro De Vita
CID (IC only):
Institution, Department, Address: Department of Physics, King's College, London.
Email: alessandro.de_vita@kcl.ac.uk
Phone: 020 7848 2715

3rd supervisor (optional)
Name: Robin Grimes
CID (IC only):
Institution, Department, Address: Imperial College London, Department of Materials
Email: r.grimes@imperial.ac.uk
Phone: 0207 594 6730

Please complete the following:

1. Project title

Modelling of stress corrosion cracking in next generation nuclear plant materials

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

Stress corrosion cracking (SCC) is a major problem for the nuclear industry. The next generation of pressurized water reactors will employ nickel alloys such as alloy 690 in much of their primary pipe work. Stress corrosion of this alloy is not well characterized and there has been virtually no modelling of this system. This project will link microscale phenomena such as crystal plasticity and grain structure effects, treated by finite element modelling, to the atomic scale crack tip processes and chemistry, treated by state of art quantum techniques In particular it will study the effect of hydrogen ingress on the bonding structure and plastic behaviour at the crack tip. Ultimately the project will be aimed at answering the question of how SCC propagates in these materials and whether crack growth rates can be predicted by modelling approaches.

1. Csanyi, G. et al. 2004. Learn on the Fly: A Hybrid Classical and Quantum-Mechanical Molecular Dynamics Simulation. Phys Rev Lett. 93 (17).
2. Kermode et al. 2008. Low speed fracture instabilities in a brittle crystal. Nature . 455, 1224-1227.
3. Wenman et al. 2008. A finite element computational model of chloride-induced stress corrosion cracking of austenitic stainless steels. Acta Mater. 56:4125-4136.

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

SCC is clearly a multi-scale problem which requires taking into account stresses, strains and plasticity at the macroscale and how these are distributed at grain level and at the crack tip. However, by the very nature of SCC (combination of stress, material and environment) any realistic analysis must also include an accurate description of the local crack tip chemistry and especially the effect of hydrogen on the crack propagation along atomic planes -since this will alter the local plasticity at the crack tip. A good indication of the feasibility of the project comes from experimental evidence showing that SCC crack tips are very sharp (~10-50 nm) and the plastic wake they leave behind, as they grow, is very small in comparison to cracks grown by other processes such as fatigue.

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

Dr Wenman is an expert in materials for nuclear applications at the macro and micro-scales, especially in metals, and he has a keen interest in finite element modelling. He has already carried out both experiments and modelling of SCC and has a background in micromechanisms of fracture.

Dr De Vita leads a research group at King's College London which is mostly devoted to the development and application of multi-scale atomistic techniques (cf. ref. 1 above on the LOTF method) to fracture problems such as catastrophic brittle fracture (ref.2) and, more recently, stress corrosion fracture, including SCC induced by hydrogen implantation. In particular, the group hosts two postdocs working on fracture problems, one of whom funded by a collaboration with Imperial College, while two new PhD students will join them in early 2010.

Prof Robin Grimes is the Head of the Centre for Nuclear Engineering at Imperial College and has 20 years experience of modelling nuclear fuel materials, especially ceramics and radiation damage, at the atomic scale. He has expertise in both molecular dynamics and density functional theory codes.

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)

Yes, the first step would be to generate a simple 2D finite element model of a crack tip, from experimental results for microstructures of these alloys, and from images of SCC crack tips in these materials. Training would also naturally involve familiarization with the multi-scale atomistic software used in King's College, shared with two new students of the local group.

This will include classical and LOTF atomistic simulations of simple fracture systems in crystalline solids.