# 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**

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Please complete the following:

*1. Project title*

Modelling dielectric losses and breakdown in polycrystalline oxides

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

We propose to study the properties of oxide films, such as MgO, $HfO_2$ and $HfSiO_4$ which are used in a wide range of electronic components: resonators for microwave communications, gate dielectric layers in metal-oxide field effect transistors (MOSFETs), and spintronic devices. As the size of these devices continually reduces, gradually reaching the nanoscale, it is becoming increasingly important to reduce their energy consumption and ensure that their reliability does not suffer. Defects, such as impurities and vacancies, often accumulate at grain boundaries in these polycrystalline materials. They contribute to dielectric loss, reducing the quality factor of microwave resonators, and provide percolation paths for electrons in MOSFETs and spintronics devices, leading to leakage and breakdown. The aim of this project is to study the properties of these defects and their response to static and THz

frequency varying electric fields using multi-scale modelling in close collaboration with experimental studies. This will involve characterizing the microstructure of polycrystalline oxide films, studying spatial distribution of defects and simulating their dynamics at finite temperature and identifying "critical events" that can lead to irreversible failure, e.g. breakdown in MOSFETs.

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

The grain microstructure will be modeled as well as the long range defect distribution within grains. The electronic and dynamics properties of individual defects within the grain and at grain boundaries will be calculated using quantum mechanical methods and inter-atomic potentials fitted to quantum mechanical molecular dynamics simulations. The embedded cluster method will self-consistently combine these methods allowing modeling defects at complex boundaries and calculating their properties in electric fields. Timescales will range from femtoseconds in electronic transitions to many years in terms of rare "critical event" models. The latter will be studied combining Monte Carlo with extremal statistics.

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

Prof. Shluger has extensive experience in the modeling of defects and grain boundaries in meal-oxide materials using quantum mechanical periodic and embedded cluster techniques [1,2]. Dr. Tangney has expertise in the development of interatomic potentials for metal-oxide systems by fitting to quantum mechanical calculations[3,4]. Prof. Alford has extensive experience in the experimental characterisation of dielectric materials and the development materials for microwave communications.

*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 – using an existing highly accurate polarizable force-field for MgO [4], the dielectric response of grain boundaries and defects in MgO will be investigated.

**References**


1. K. P. McKenna and A. L. Shluger, "The interaction of oxygen vacancies with grain boundaries in monoclinic $HfO_2$," - Appl. Phys. Lett., 95, 222111 (2009).
2. A. L. Shluger, K. P. McKenna, P. V. Sushko. D. Munoz Ramo, A. V. Kimmel, "Modelling of electron and hole trapping in oxides," Mod. Simul. Mater. Sci. Eng. 17, 084004 (2009).
3. P. Tangney and S. Scandolo, "An ab initio parametrized interatomic force-field for silica" J. Chem. Phys. **117** 8898 (2002)
4. P. Tangney and S. Scandolo, "A many-body interatomic potential for ionic systems: application to MgO," J. Chem. Phys. 119, 9673 (2003).