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: Dr Daniele Dini
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2nd supervisor
Name: Professor Mike Finnis
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3rd supervisor (optional)
Name: Professor David M. Heyes
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Please complete the following:

1. Project title **Atomistic-continuum hybrid coupling to model nano-indentation of metal films**

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

The mechanics and dynamics that govern contact interfaces range from atomic- to macro-scale phenomena. Surface physicists and engineers have known the importance of analysing all the relevant scales together and linking them properly for many years and it has now become crucial to understand the relationship of processes taking place across various length and time scales for the advancement of various fields like material science, micro and nano technology, biology.

The difficulty in resolving interfacial "mysteries" (e.g. there still is no universally accepted explanation of the basic laws of friction) is due to the multi-scale nature of the phenomenon. Molecular and atomistic interactions influence the macroscopic behaviour, and are themselves affected by the macroscopic configuration. Traditionally, the various scales of the problem have been tackled independently. For instance, the macroscopic behaviour of systems is predicted from continuum based theory and computational models, which

traditionally have phenomenological constitutive relationships. But the macroscopic behaviour is inherently governed by the physics taking place on multiple unresolved scales.

The aim of this project is to build a hybrid computational framework which would enable to bridge the gap between atomistic and continuum simulations. The development of a concurrent atomistic-continuum coupling method is envisaged based on a blending of the continuum stress and the atomistic force in the equilibrium equation. The solver will be tested on the nano-indentation of thin metal films, where the domain of interest will decomposed into continuum, atomistic, and overlap sub-domains with a blended atomistic–continuum description, where compatibility between the atomistic solution and the continuum solution is imposed within the overlap region in a weak sense. The atomistic description will be obtained using molecular dynamics [1] and the potentials used to characterise the metal films will range from simple LJ to Finnis-Sinclair [2] to EAM. The continuum will be modelled as linear elastic using FEM and/or BEM.

[1] Heyes, D.M., T.A. Zaki, and D. Dini, "Non-Equilibrium Molecular Dynamics Simulations of Shear Characteristics in Dry and Lubricated Contacts", in Proceedings of the World Tribology Congress 2009 (WTC IV), Kyoto, 6-11 September 2009.
[2] Sinclair J.E. and Finnis, M.W. (1984) "A simple empirical n-body potential for transition metals", Philosophical Magazine A, **50**, pp. 45-55.

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

The project is inherently multi-scale! At the atomic scale atomistic simulations will be used to capture the non-linearities induced by the nano-indentation process, such as dislocation nucleation. At the larger length scale, the atomistic details will be replaced by the continuum description (see Figure 1).

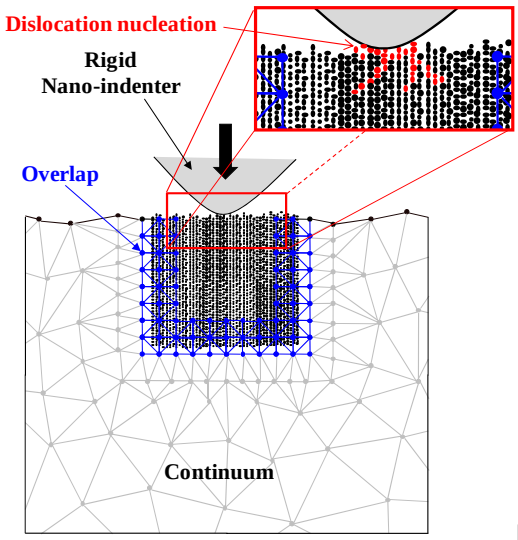

Figure 1.

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

Dr Dini's expertise is in continuum computational mechanics and he has developed a number of analytical and numerical methods for the solution of advanced contact problems. Professor Heyes is an expert in molecular dynamic simulations and has been recently

developing, together with Dr Dini, an *ad hoc* MD code to model tribological interactions. Professor Finnis is a world-leader in the development of metal potentials for atomistic simulations. The blend of skills is ideally suited to guarantee the success of the proposed project.

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. A suitable project would involve the development of atomistic simulations of nano-indentation of thin films using different potentials (i.e. LJ, Finnis-Sinclair, EAM) to describe the metallic characteristic of the film (Al, Ni, Cu could be used as reference materials).