Application for a TSM-DTC funded PhD studentship

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

1st supervisor
Name: M. W. Finnis
CID (IC only): 461974
Institution, Department, Address: Department of Materials and Department of Physics, Imperial College London, Exhibition Road, London SW7 2AZ
Email: m.finnis@imperial.ac.uk
Phone: +44 (0) 207 59 46812

2nd supervisor
Name: A. De Vita
CID (IC only):
Institution, Department, Address: Department of Physics, King's College London, Strand, London, WC2R 2LS
Email: alessandro.de_vita@kcl.ac.uk
Phone: +44 (0) 207 84 82715

3rd supervisor (optional)
Name: P. D. Lee
CID (IC only):
Institution, Department, Address: Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ
Email: p.d.lee@imperial.ac.uk
Phone: +44 (0) 207 59 46801

Please complete the following:

1. Project title: Interfacial free energy of solid-melt interfaces in light metals and alloys

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

Successful modelling of casting depends on parameters such as the solid-liquid interfacial free energy and solidus-liquidus compositions. The project will provide theoretical thermodynamic data of this kind, based on atomic scale calculations. Advanced light alloys composed mainly of aluminium, magnesium and calcium are of strategic importance for e.g., modern aerospace and transport technologies. We shall focus on these three metals.
We divide the project into three phases:
i). Derivation of accurate, classical potentials based on ab initio data. We shall start with ab initio, density-dependent pair potentials (pp,183-185 of Finnis[1]), however, interatomic forces in Ca are complicated by d-states near the Fermi energy, demanding a more sophisticated treatment. A correction function for all the metals will be derived using the recent information-theoretic approach of Bartók et al[2], making highly efficient use of ab initio data[3].

ii). Calculation of liquid-melt interfacial energies for the pure metals can then proceed with our metadynamics approach[4].
iii). Parts of the two-component phase diagrams will be compared with predictions of the new models as well as with commercial CALPHAD software (i.e. ThermoCalc, www.thermocalc.com). The influence of the new values on predicted solidification structures will be tested using existing public domain microstructural codes. (e.g. http://www3.imperial.ac.uk/advancedalloys/software).

3. What is the multi-scale nature of the project? (≤ 100 words please)
There are three scale-bridging operations: the derivation of a potential function to represent total energies, the computation of thermodynamic quantities such as interfacial free energy and the demonstration of the impact of these calculations on microstructural predictions.

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)
Finnis has experience of ab initio pair potentials and ab initio calculations generally, and supervised the metadynamics work on solid-liquid interfacial free energy, De Vita works on multiscale materials modelling[5] and is currently working with Csanyi on implementing the Bartók et al approach for silica, and Lee is expert in the alloy properties and key quantities of engineering interest and their influence on microstructure formation.

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 (derivation of a density-dependent pair potential for Mg).

1. Finnis, M. W., *Interatomic Forces in Condensed Matter*. OUP: Oxford, 2003.
2. Bartók, A. P.; Payne, M. C.; Kondor, R.; Csányi, G., Gaussian Approximation Potentials: the accuracy of quantum mechanics, without the electrons. *arXiv:0910.1019v3 [physics.comp-ph]* **2009**.
3. Pártay, L. B.; Bartók, A. P.; Csányi, G., Full sampling of atomic configurational spaces. *arXiv:0906.3544v1 [cond-mat.stat-mech]* **2009**.
4. Angioletti-Uberti, S.; Ceriotti, M.; Finnis, M. W.; Lee, P. D., Solid-Liquid Interface Free Energy through Metadynamics Simulations. *arXiv:0911.2615v1* **2009**.
5. Makov, G.; Gattinoni, C.; De Vita, A., Ab initio based multiscale modelling for materials science. *Modelling Simul. Mater. Sci. Eng.* **2009,** *17*, 084008.