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: Paul Tangney

CID (IC only): 523935

Institution, Department, Address: Imperial College London, Department of Materials, London SW7 2AZ

Email: p.tangney@imperial.ac.uk

Phone: 020 7594 8155

2nd supervisor

Name: Alessandro De Vita

CID (IC only):

Institution, Department, Address: King's College London, Department of Physics, London WC2R 2LS

Email: alessandro.de_vita@kcl.ac.uk

Phone: 020 7848 2715

3rd supervisor (optional)

Name: Robert Zimmerman

CID (IC only): 00154591

Institution, Department, Address: Imperial College London, Department of Earth Science and Engineering, London SW7 2AZ

Email: r.w.zimmerman@imperial.ac.uk

Phone: 020 7594 7412

Please complete the following:

1. Project title

The Chemo-mechanics of Fracture in Earth Crust Minerals.

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

In a world increasingly famished for commodity materials, the industrial processes involved in extracting useful materials from earth crust minerals are a cause of growing concern. Mining stands easily among the most energy-intensive human activities. While known ore bodies become exhausted, and novel reserves get progressively more difficult to locate, extract and process, traditional techniques used to extract and comminute rocks will have an increasingly severe environmental impact, and raise ever more serious sustainability issues. Strikingly, however, many processess occurring in fracturing rocks are still not understood (ref. 1), and in particular our current level of understanding of the fracture process at an atomistic length scale is, at best, poor, in spite of the potentially huge economic and environmental impact of the new technologies which such knowledge would be likely to generate.

The present project will make a step in the right direction by showing that accurate simulations of mineral fracture can be made practicable, by combining a quantum mechanical description of the crack tip with a classical atomistic model that captures the long-range elastic relaxation of the surrounding crystal matrix. A classical potential specially tailored for electrostatically complex mineral materials (ref. 2) will be used within a QM/MM technique (refs. 3,4) to investigate two classes of processes which may concertedly drive the fracture of silicates exposed to an aggressive environment. These are (i) failure at chemically weak points due to diffusion and segregation of mineral matrix components such as alkali ions, and (ii) localized chemical attack by aggressive species at the interface between minerals and liquid phases such as H_2O containing O_2.

Very large model system sizes are envisaged throughout the project, making a multi-scale simulation approach, and massively parallel computing, mandatory. An attempt will be made to derive from these results macroscale constitutive equations and failure criteria usable in macro-scale simulations.

References

1. Jaeger JC, Cook NGW, Zimmerman RW. *Fundamentals of Rock Mechanics, 4th ed.* Wiley-Blackwell, 2007.

2. Tangney P, Scandolo S. An ab initio parametrized interatomic force field for silica. *J. Chem. Phys.* **117** 8898 (2002)

3. Csanyi, G. et al. Learn on the fly: A hybrid classical and quantum-mechanical molecular dynamics simulation. *Phys Rev Lett*. **93** 17550 (2004)

4. Kermode et al. Low speed fracture instabilities in a brittle crystal. *Nature*. **455**, 1224-122 (2008)

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

Fracture is perhaps the archetypical multiscale system: the conditions for crack propagation are created by the concentration of a long-range stress field at an atomically sharp crack tip, creating a complex and strongly coupled multiscale system. An accurate, quantum mechanical, description of the chemical processes taking place at the crack tip is therefore essential. For the results of these simulations to become technologically useful, however, they must eventually be expressed in terms of macroscale constitutive equations and failure criteria that can be used in mine-scale or mill-scale numerical simulators – roughly ten orders of magnitude larger than the length-scale of the crack tip.

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

Dr Tangney is an expert on the development of novel classical interatomic potentials which encapsulate knowledge of the electronic degrees of freedom of the underlying physical system, for example by including an explicit representation of ionic dipole moments (ref. 2 above).

Dr De Vita works in King's College London on the application of multi-scale atomistic techniques to fracture problems. His group includes a postdoc, Dr James Kermode, developing methodologies and modelling tools to investigate mineral systems.

Prof. Zimmerman is an expert on continuum-scale rock mechanics, including elasticity, plasticity and fracture. He works in Imperial College's Department of Earth Science and Engineering Department, where he leads the Rock Fragmentation Project within the Imperial College Center for Advanced Mineral Recovery, funded by the UK-based mining giant Rio Tinto.

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, there are actually two alternatives, depending on the interests of the student:

(i) Carry out a few large-scale, purely classical, simulations of the catastrophic brittle fracture of a crystalline material. This would serve as an introduction both to fracture mechanics and to the practicalities of running computational experiments, without yet incurring the high cost of massively parallel QM calculations.

(ii) Apply for the first time an enhanced classical potential including metal ions, e.g. magnesium and aluminium, to allow more complex minerals such as alkali feldspars to be modelled. This

would require representative DFT calculations to be carried out to test the accuracy of the new potential, and would give a good overview of the major techniques - DFT and classical MD - required for the project.

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[1] This excludes some forms of matter such as gases and solid argon, but it does not exclude liquids, such as those used in melt processing, liquid crystals, or novel ionic liquids. The crucial point is that there is some technology that the material already enables or may enable in the future.