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
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Please complete the following:

1. Project title

Phase stability in biomedical Ti alloys

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

In recent years there has been much interest in the development of low modulus, biocompatible bcc titanium alloys for biomedical applications including arterial stents, hip replacements and fixation plates [1]. Relevant observations include (i) the decrease in C' with electron per atom ratio [2], (ii) the vulnerability of some alloys to precipitation of the ω and α'' phases [3] due to the softening of phonons in the shear transformation directions, (iii) the stabilization by oxygen of the bcc structure with respect to these phonon modes [4]. This produces a number of exciting opportunities for the development of shape memory or high strength biomedical Ti alloys. The project will involve (i) describing the interplay between Nb, Zr and Ta substitutions on the enthalpy, phonons and elastic constants of the β, ω, α'' and α phases, (ii) the effect of O additions between 0-2 at% and (iii) simulations of the interface energies, all using DFT. These effects will then be combined in either a crystal plasticity finite element model (CPFEM) or an Eshelby composite model for a polycrystal

[elastic-plastic self-consistent (EPSC) model] to produce an overall model of the shape memory / superelastic response to stress. The project will span length-scales from sub-nm to mm.

[1] Saito *et al*. "Multifunctional alloys obtained via a dislocation-free plastic deformation mechanism." *Science* (2003) **300** (5618) pp. 464-467.
[2] Talling *et al*. "Determination of (C-11-C-12) in Ti-36Nb-2Ta-3Zr-0.3O (wt.%) (Gum metal)." *Scripta Materialia* (2008) **59** (6) pp. 669-672.
[3] Talling *et al*. "On the mechanism of superelasticity in Gum metal." *Acta Materialia* (2009) **57** (4) pp. 1188-1198.
[4] Petry *et al*. "Phonon dispersion of the bcc phase of the group-IV metals. I. bcc titanium." *Physical Review B* (1991) **43** pp. 10933-10947; Varma and Weber. "Phonon-dispersion in transition metals." *Physical Review B* (1979) **19** (12) pp. 6142-6154.

3. What is the multi-scale nature of the project? (≤ 100 words please)
First principles density functional theory calculations will be used to supply interface energy (assumed small in the first instance), Gibbs energy and modulus terms to an Eshelby composite model for each individual grain in the self-consistent approach, for the prediction of shape memory and superelastic properties as a function of composition. The lengthscales therefore span from atomistic (sub-nm) to thousands of grains (~1mm).

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)
PDH – first principles DFT
DD – experimental and numerical micromechanics
MWF – thermodynamics and empirical potentials

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 key question is whether the effect of O interstitials can be considered as simply a size effect or if the chemical nature of the bonding is important. In order to distinguish between these two possibilities, it is proposed to add a empirical force field to the DFT calculation of the relaxed Ti structures to mimic the size effect of an O interstitial without including any chemical interaction, and to compare both to pure Ti and Ti with an O addition. This will give the student some experience with modifying the code and start getting them involved in the issues at the heart of the project.