Application for a TSM-DTC funded PhD studentship

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and submit to (l.wanjohi@imperial.ac.uk)
by Friday January 8, 2010

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Please complete the following:

1. Project title
Developing vacancy and dislocation motion models to predict the enhanced healing of voids during the thermomechanical processing of advanced alloys

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

During the processing of advanced alloys voids form on a range of scales from nanometer to micron, which ideally are healed during subsequent thermomechanical processing. However, many of these voids persist and are highly detrimental to the final properties of advanced alloys used in aerospace and power applications. The healing process occurs due to macroscopic stress and strain causing local flow and diffusion of atoms/vacancies closing the pores. The rate of diffusion is very dependent on the vacancy and dislocation mobility, which are coupled. This project will first develop 2D models of vacancy and dislocation motion as a function of the local stress state in the presence of voids and as a function of the macroscopic stress state; 3D modeling may also be carried out. Void formation will then be modeled on a continuum scale and the relationships developed at the dislocation mechanics scale will be incorporated to predict void healing. The simulations will be validated via

comparison to in situ observations obtained from previous studies of void healing during deformation (no experimental work will be carried out in this project).

References

Defect formation and damage growth models:

- Phillion, A.B., Cockcroft, S.L.; Lee, P.D., "Predicting the constitutive behavior of semi-solids via a direct finite element simulation: application to AA5182", Modelling Simul. Mater. Sci. Eng. 17 (2009) 055011 (15pp). doi:10.1088/0965-0393/17/5/055011
- Lee, P.D., Chirazi, A., Atwood, R.C. and Wang, W., "Multiscale modelling of solidification microstructures, including microsegregation and microporosity, in an Al-Si-Cu alloy", Mat. Sci. Eng. A, 365 (1-2), 57-65, 2004.
- Youssef Y.M., Chaijaruwanich, A., Hamilton, RW, Nagaumi, H, Dashwood, RJ, Lee, PD, "X-ray microtomographic characterisation of pore evolution during homogenisation and rolling of Al–6Mg", Mat. Sci. Tech. 22 (9), 2006, 1087-93
- Chaijaruwanich, A., Dashwood, RJ, Lee, PD, and Nagaumi, H, "Pore evolution in a DC cast Al – 6 wt% Mg alloy during hot rolling", Acta Mat., 54, 2006. 5185–94.
- A. D. Foster, J. Lin, D. C. J. Farrugia and T. A. Dean, 2007, An Investigation into Damage Nucleation and Growth for a Free-Cutting Steel at Hot Rolling Conditions, *J. of Strain Analysis.* Vo 42, pp227-235. DOI: 10.1243/03093247JSA230*.*
- A. D. Foster, J. Lin, D. C. J. Farrugia and T. A. Dean, 2009, A test for evaluating the effects of stress-states on damage evolution with specific application to the hot rolling of free-cutting steels. To appear in *Int J of Damage Mechanics*
- W. Zhuang and J Lin**,** 2008, An integrated micromechanics modelling approach for micro-forming simulation, *Int. J. of Modern Physics B (IJMPB)*, Vol. 22, Issue 31/32, **pp**5907-5912. DOI: 10.1142/S0217979208051352

2D discrete dislocation modeling of polycrystals:

- Balint, DS, Deshpande, VS, Needleman, A, et al., Discrete dislocation plasticity analysis of the grain size dependence of the flow strength of polycrystals, INT J PLASTICITY, 2008, Vol: 24, Pages: 2149 – 2172.

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

The main focus of the project will be developing models of dislocation and vacancy motion. Dislocation/diffusion modeling will be carried out at the nano scale. The understanding of the physical behavior of the material via the nano-scale modeling will be used for the development of crystal plasticity material models for micro-mechanics modeling techniques. The material models will be embedded in a macro-scale finite element model usable by the steel industry.

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

Balint is an expert on developing dislocation models at the nano scale. Lee is an expert on front tracking simulations (and experimental investigations) of defect formation at the microstructural scale. Lin is an expert on crystal level plasticity, macroscopic behaviour of metals and constitutive behaviour definition for a wide range of metal forming processes. Their expertise therefore spans both a range of physical phenomena (atomisitic/dislocation mechanics, diffusive/reactive/fluid flow, and stress analysis) and scales from nanometer to millimeter.

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 several distinct portions of this project that could be easily encapsulated into a 12-week MSc. For example, during a 12-week MSc the student could develop a 2D model of dislocation dynamics and dislocation interactions with surfaces, and then estimate how that enhances surface self-diffusivity of the alloy.