Institution: University of Greenwich

Unit of Assessment: (UoA 13) – Electrical and Electronic Engineering, Metallurgy and Materials

Title of case study: Advanced Materials Modelling for Earth and Space Application

1. Summary of the impact

Research in materials modelling by the Computational Science and Engineering Group (CSEG) is helping aerospace, defence and transport companies design advanced materials and new manufacturing processes. From lightweight components like aeroengine turbine blades to the control of magnetic fields to stabilise the next generation of International Space Station levitation experiments, CSEG is supporting innovations which have:

- economic impact due to increase in competitiveness, market share, energy cost reduction and better use of raw materials;
- environmental impact due to new lightweight recyclable materials and reduced energy processes;
- increased public awareness of the importance of advanced materials and influenced government policy.

In the assessment period, CSEG collaborated closely with leading industries in steel-making (ArcelorMittal, Corus), primary aluminium (Dubal, Rusal, Norsk-Hydro, SAMI) and lightweight structural materials for transport and aerospace (European Space Agency, Rolls-Royce).

2. Underpinning research

The CSEG at the University of Greenwich, led by Professor Pericleous and currently including Bojarevics, Djambazov, Kao (2010-) and Patel, develops advanced numerical modelling tools and software and provides process solutions to experimental researchers and industrial end-users. The group simulates the life-cycle of materials from their fundamental properties to extraction methods, to processing use in advanced manufacturing, to failure characteristics and recycling. It traces materials research to the 1980s with HiSmelt (1985-2003, '*at Aus$1billion Australia's largest privately funded research project*'), a direct smelting process making iron straight from the ore. HiSmelt was developed from the start using Computational Fluid Dynamics modelling that led to the development of FV code PHYSICA [3.1, 3.2]. It pioneered the term "Multi-Physics" modelling in the mid-1990s with further development of PHYSICA through the *ACME Casting Initiative: Numerical Modelling* (GR/G36265) and *Multi-Physics Numerical Modelling of the Casting Process* (GR/K42370), with Pericleous and Bailey as co-investigators [3.2] (the PI, Prof Mark Cross, left in 2005).

These early beginnings, including collaboration with Professor John Campbell's casting group in Birmingham, led to advanced materials research for transport and aerospace (particularly titanium-based alloys [3.3]). To this end, CSEG collaborated with several end users: BAe, Rolls-Royce, Qinetiq, the European Space Agency (ESA), Wiggins Special Metals, Phoenix Scientific Industries, and with academics at Birmingham, Brunel, Imperial College, Leeds and Swansea. Relevant EPSRC support came in a stream of linked projects GR/L97483/01 [3a](1998), GR/N14316/01 [3b] (2001), EP/D505011/1 [3c] (2006-2009); EU support (eg the €40M FP6-IP intermetallics project IMPRESS [3d], 2005-2010) and the TSB/MoD titanium powder project COLDMELT [3e] (2008-2011). Support continues with EP/K00588X/1 [3f] (2012) "UltraMelt" and the production of magnesium/aluminium Metal_Matrix_Nano_Composites (MMNC), using external force fields in EXOMET [3g] (€19M-EU-FP7). These projects target the manufacture of lightweight alloy components for aeroengines (blades, discs), fuel tanks for spacecraft, copper wiring replacements, suspension links for cars etc.

A strong vein running through this research features the application of magnetic fields to control the melting, flow and solidification of alloys (Ti, Si, Al, Zr) [3.4] that are highly reactive as liquids and, as a useful corollary, to simulate microgravity conditions for property measurement experiments [3.5]. Accurate spectral software was specifically developed to model flow, heat transfer and solidification in levitated conducting liquids with dynamically varying free surfaces, within an imposed electromagnetic (EM) field. This code, SPHINX (Bojarevics, Pericleous) [3.4], has been used for thermophysical property studies underpinning the projects listed, and in the ESA ELIPS-3 [3h] materials projects (THERMOLAB-ISS and PARSEC). Comparative studies between terrestrial and microgravity methods for thermophysical property measurements have been carried out in collaboration with the National Physical Laboratory, the German Aerospace Research Establishment (DLR) and the high magnetic field laboratory in Grenoble. Modelling highlighted the importance of static magnetic field damping to counteract gravity effects in measurements, leading to simulations for ASTRIUM to stabilise the next generation of International Space Station levitation experiments.

Magnetic field influence on alloy microstructure [3.6] has been observed, but never explained fundamentally. With the prospect of advancing a new microstructure control mechanism, we are studying this phenomenon theoretically and experimentally, with Manchester University and Diamond (the UK Synchrotron facility) as collaborators (EPSRC EP/K011413/1 [3j] "*TECalloy*", 2013).

3. References to the research (REF1 submitted staff in **bold**, **REF2 Output)

3.1 Croft, N., Pericleous, K., & Cross, M. (1995). PHYSICA: a multiphysics environment for complex flow processes. *Numerical methods in laminar and turbulent flow*, *9*(Pt 2), 1269–1280.

3.2 Bailey, C., Chow, P., Cross, M., Fryer, Y., & Pericleous, K. (1996). Multiphysics Modelling of the Metals Casting Process. *Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences*, *452*(1946), 459–486. http://dx.doi.org/10.1098/rspa.1996.0024

3.3 Wang, H., **Djambazov, G., Pericleous, K. A., Harding, R. A., & Wickins, M. (2011). Modelling the dynamics of the tilt-casting process and the effect of the mould design on the casting quality. *Computers & Fluids*, *42*(1), 92–101. http://dx.doi.org/10.1016/j.compfluid.2010.11.010

3.4 Bojarevics, V., Pericleous, K., Harding, R. A., & Wickins, M. (2004). The development and experimental validation of a numerical model of an induction skull melting furnace. *Metallurgical and Materials Transactions B*, *35*(4), 785–803. http://dx.doi.org/10.1007/s11663-004-0019-3

3.5 Bojarevics, V., & Pericleous, K. (2003). Modelling electromagnetically levitated liquid droplet oscillations. *ISIJ international*, *43*(6), 890–898. http://dx.doi.org/10.2355/isijinternational.43.890

3.6 Bojarevics, V., **Kao, A**. and Pericleous, K. (2012) Modeling the Fluid Dynamics and Dendritic Solidification in EM-Levitated Alloy Melts. In D. M. Herlach and D. M. Matson (Eds.). *Solidification of Containerless Undercooled Melts*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany. http://dx.doi.org/10.1002/9783527647903.ch15

Relevant Grant Information (*Prof Pericleous is the PI unless otherwise stated*)

3a EPSRC **GR/L97483/01**(1998-2001), £139,324 – "*Containerless melting of reactive metals for castings of the future*" ; **Rating:** Tending to Outstanding

3b EPSRC **GR/N14316/01**(2001-2003), £135,514 – "*Net-shape casting of TiAl components*", **Rating:** Tending to Outstanding

3c EPSRC **EP/D505011/1**(2006-2009), £169,188 – "*Measurement and modelling of electrical, transport and phase-change phenomena and application to Vacuum Arc Remelting*";

3d EU/ESA FP6-IP, NMP3-CT-2004-500635 "IMPRESS" (2005-2010), €41M total, €600k UG, "*Intermetallic Materials Processing in Relation to Earth and Space Solidification*"

3e TSB/MoD TP #100441 (2008-2012), £141,282 "COLDMELT - *Cold wall melting and pouring of titanium*"

3f EPSRC **EP/K00588X/1**(2013-2016), £281,797 "UltraMelt - *Fundamental Study of Cavitation Melt Processing: Opening the Way to Treating Large Volumes*"

3g EU/ESA FP7 NMP3-LA-2012-280421 "EXOMET" (2012-2016), €19M total,€400k UG, "*Physical processing of molten light alloys under the influence of external fields"*

3h ESA ELIPS-3[#] materials projects (2010-2013): THERMOLAB-ISS #AO-2009-1020: "*Thermophysical properties of liquid metallic alloys – modelling of industrial solidification processes and development of advanced products"* and PARSEC #AO-2009-0262 "*Peritectic Alloy Rapid Solidification with Electromagnetic Convection"*

[#] Internally funded due to lack of UK funds for materials microgravity projects

3i Royal Society Int. Exchanges Scheme – China (NSFC) (2012-2014), £9669 "*Thermo-electromagnetic convection on dendritic growth kinetics in undercooled melts*"

3j EPSRC **EP/K011413/1**(2013-2016), £278,790 "*TECalloy - Disruptive Solidification Microstructures via Thermoelectric Control*"

3k EU FP7-ENV-2013 grant #603718 "SIKELOR" (2013-2017), €234k, Bojarevics (PI), "Silicon Kerf Loss Recycling"

4. Details of the impact

During the assessment period, the group assisted many aerospace, defence and transport companies to optimise materials processing and component manufacture, and enhance product reliability. Impacts from this interaction include:

a) the introduction of new manufacturing methods through design, plus change of practice or policy through greater understanding;
b) environmental impact due to new lightweight recyclable materials, reduced energy processes and CO_2 emissions;
c) economic impact due to increase in competitiveness, market share, reduction in energy costs and better use of raw materials.

Impact by activity:

- **Intermetallics**: our modelling was instrumental in the success of the pan-European IMPRESS [3d] project[1] (2005-2010), for the manufacture and use of intermetallics and developing a process route for the melting and casting of γ–TiAl turbine blades[1] which re-orientated materials development for the next generation of Rolls-Royce aeroengines. Quoting Wayne Voice (then RR section head) at the TiAl symposium, Birmingham 2010: "W*ithin a decade, high efficiency aero-engines will feature lightweight TiAl instead of nickel superalloy blades.*" Casting of thin blades requires high superheat; we devised a new method of increasing superheat in cold crucibles using static magnetic field damping (LMPC best paper award). This was confirmed experimentally by Consarc (the furnace manufacturer) that patented the idea (2011)[2]. In the same framework, we modelled gas atomisation to assist the development of novel Raney (NiAl) metal powder catalysts. These found use in hydrogen fuel cells (Oy Hydrocell Finland) and as platinum replacement catalysts (Johnson Matthey). To inform the general public of these environmentally important advances, a Materials Challenge Exhibit was set up at the London Science Museum and a web-streaming lecture by Pericleous on Modelling the Melting and Casting of TiAl Turbine Blades was recorded by ESA.

  >*This activity demonstrates (1)***economic impact** *for the companies mentioned, (2)***Impact on the environment** *with the production of lightweight aerospace materials and low cost catalysts, (3)* **Impact on society** *through public engagement in a museum exhibit and a web lecture informing the products of research.*

- **Our multi-physics codes** (PHYSICA, SPHINX) have been used elsewhere: *by Qinetiq* for EM-induction-assisted titanium forging; *by ArcelorMittal (France)*, licensed (2009) to improve understanding of the continuous casting of steel plate (work that won the *Association Technique de la Siderurgie* award[3]), and to improve efficiency of the Basic Oxygen Converter (2012); *by Corus (NL)* for a novel levitation melting and evaporation process of zinc in steel plate coating – a process successfully sold to Pohang Steel in Korea (2009); *by Corus (UK), Wiggins Special Metals and Rolls-Royce* to understand defect formation in Vacuum Arc Remelting for aerospace quality steel and titanium ingots [3c] (2010).

  >*This activity demonstrates* **economic impact** *for Corus (development of novel coating process) and ArcelorMittal (better understanding and optimisation of steel production).*

- **Primary aluminium production**: our *shallow-layer* code MHD-VALDIS (£120k licence sales 2008-2013) computes MHD stability in aluminium production smelters, helping organisations worldwide with the design and optimisation of the latest production cells: Rusal[4] (Russia), Dubal (Dubai), Norsk Hydro (Norway), Wireless Technologies[5] (US), GAMI and SAMI, China. The latter two (allied to Chinalco), compete for the largest cells in the world at 500kA (2013). Close liaison with aluminium smelter designers reduces electricity use and CO_2 emissions in this energy-intensive process.

>*This activity demonstrates (1)***economic impact** *to Greenwich Enterprise Ltd, Wireless Technologies and aluminium plant operators (2)***Impact on the environment** *due to reduction in carbon usage and energy requirement in large aluminium production plants.*

- **Microgravity**: models require accurate material properties. Our ability to model in detail the dynamic interaction of externally imposed electromagnetic fields and levitated metals attracted the thermophysical property measurement community for high temperature melts, under terrestrial or microgravity conditions. This led to collaborations with ESA, NPL (UK), DLR (Germany), SIMAP[6] (France) and ASTRIUM[7] (Germany). We are currently the only UK institution taking part in the European Space Agency ELIPS-3 [3h] materials programme (projects PARSEC, Thermolab-ISS, SOL-EML) in the company of NASA, JAXA (Japan) and DLR (Germany). As an outcome, Prof Pericleous was invited to make a case for UK funding of materials space research, to joint UK Space Agency/EPSRC meetings (July 15 and Nov 7 2012[8]). This successful appeal led to a ministerial decision to make UK funding available for ELIPS-4 projects.

  > *This activity demonstrates* ***impact on policy***.

- **Titanium powder**: TSB activity (project COLDMELT [3e]) in collaboration with PSI[9], gives UK a lead in the production of titanium powder for aerospace components. Dual frequency electromagnetic fields are used to produce clean, inclusion-free melt-stream for gas atomization, using a contactless nozzle and a novel high-capacity holding crucible. The furnace is still being assembled, but components of the design are already exported to overseas installations.

  > *This activity demonstrates (1)***economic impact** *for PSI ltd in the production of a strategic aerospace/defence material, income and employment generation*

- **MMNCs**: the production of light alloy Metal-Matrix-Nano-Composites is seen as a way to reduce the weight of transport and aerospace structures. External fields (acoustic, magnetic) assisting the distribution of micro/nano particles, form the theme of FP7 EXOMET [3g] that employs our models. Participating industrials include Volvo, EADS, Fiat, AVIO and ALD. A European patent application has been submitted jointly with ALD and ESA[1] to protect a novel contactless EM vibration coil designed by us, for particle de-agglomeration and dendrite fragmentation in liquid metals during solidification.

5. Sources to corroborate the impact

1. Head of New Materials & Energy Unit, European Space Agency.
2. National Exploration and Microgravity Programme Manager, UK Space Agency.
3. Managing Director, Phoenix Scientific Industries (PSI) Ltd.
4. CEO, Wireless Industrial Technologies Inc.
5. Head of Modelling Group, RUSAL
6. Consarc patents - http://www.patentgenius.com/patent/7167501.html (2007) and http://www.faqs.org/patents/app/20110075697 (2011), *regarding use of DC fields to increase superheat in cold crucible melts*
7. **Metallurgical and Materials Transactions B**, Vol. 44, Issue 3, pp 653-670, June 2013; Journal paper to verify contributions to steelmaking for ArcelorMittal
8. SIMAP reference: **High Temperature Materials and Processes**, 27 (6). ISSN 0334-6455
9. For microgravity research ***JOM: Journal* of the Minerals, metals, and Materials Society - Springer** (JOM), 2012, Vol. 64, No. 9, pp. 1089-1096