Institution: Loughborough University

Unit of Assessment: B10 Mathematical Sciences

Title of case study: Increasing technological capability and reducing development costs in the manufacturing of surface coatings and structures

Period when the underpinning research was undertaken: 2005 – 2020

Details of staff conducting the underpinning research from the submitting unit:

Name(s):	Role(s) (e.g. job title):	Period(s) employed by submitting HEI:
A. J. Archer	Professor of Applied Mathematics and Theoretical Physics	2006 – present
R. Smith	Professor of Mathematical Engineering	1972 – present
D. Tseluiko	Senior Lecturer	2010 – present
D. Sibley	Senior Lecturer	2015 – present

Period when the claimed impact occurred: 1st August 2013 - 2020

Is this case study continued from a case study submitted in 2014? N

1. Summary of the impact (indicative maximum 100 words)

Depositing materials on surfaces to form thin coatings and microscale structures is a crucial aspect of modern high-tech manufacturing, but there are challenges to be overcome to make such processes feasible. Loughborough mathematical modelling has, through greatly broadening their capacity and knowledge, and by guiding their decisions in ways that save time and money, brought **economic benefit** to two international companies developing such processes. In particular, our collaboration with M-Solv Ltd, a UK-based global developer and manufacturer of micromachining and micro-deposition equipment, has enabled them to develop an inkjet printing process for producing electrical connections on touchscreens and solar-panels. Similarly, collaboration with AGC (Asahi Glass Co.), the top global glass manufacturer, has enabled the development of new film coatings on window glass to improve heat-retention.

2. Underpinning research (indicative maximum 500 words)

Automated fabrication of small-scale surface coatings and structures is an integral part of modern manufacturing. However, there are difficulties to be overcome in developing such processes, which the Mathematical Modelling research group at Loughborough has a strong history of impacting on. We have performed multiscale modelling of inkjet printing and sputter deposition on surfaces, applying a variety of techniques that span from continuum to discrete models, to impact the development of new manufacturing machinery and processes of two international companies, M-Solv Ltd and Asahi Glass Co.

Modelling for inkjet printing

On non-porous surfaces ink (i.e. a suspension of particles in a volatile liquid) can move significantly whilst it dries. Coarse-grained Kinetic Monte Carlo (KMC) models for drying on non-uniform and/or rough surfaces were developed [**R1, R3**], which enabled us to advise M-Solv Ltd on what strategies to use when printing for manufacturing electrical connections with inks containing conducting metal particles. These are used in making the connections on solar panels and touch screens. This KMC model was complemented by Dynamical Density Functional Theory (DDFT) based modelling [**R2**], for speed, larger systems and deeper understanding of the ink phase behaviour.

The coarse grained KMC models are based on a discretisation of the liquid onto a grid of lattice points and then using Monte Carlo methods to evolve in time the locations on the lattice of the coarse-grained "particles". DDFT is a theory for the time evolution of the density distribution of the liquid molecules. Such particle resolved models allow us to track where in the system both the liquid and the ink particles move to over time, allowing for fundamental understanding of the processes occurring as the ink moves over the surface during drying. They are particularly useful for modelling liquids on heterogeneous and structured surfaces.

Modelling for sputter deposition

Low-emissivity coatings on window glass are manufactured by depositing multilayer nanoscale thin films by magnetron sputtering. To understand the nanoscale features, the Loughborough team developed atomistic adaptive KMC (a-KMC) models. Simpler approaches, such as the commonly used molecular dynamics (MD) computer simulation type models cannot be used because MD cannot access the experimental time scales. MD can at best only describe the film growth for a few microseconds. To model the growth of the full film with MD, one must set the material deposition rate to be unrealistically fast. The a-KMC technique involves determining adaptively the location of saddle points surrounding local minima in a $3N$-dimensional phase space [**R4**], where N, the number of atoms involved, can be in excess of 1000. This allows the deposition onto the surface and the diffusion of the particles over the surface to be modelled and thus the growth of thin films over experimental timescales to be described. Typical experimental growth times are between 1 and 10 monolayers per second. Our technique allows simulations of deposition over seconds to be done. Publications [**R4**–**R6**] give details of the underpinning research being applied to problems of significance to AGC. In [**R4**] the long-time dynamics simulation model was developed and applied to the growth of silver and aluminium films. The method was further developed in [**R5**] to study the growth of silver films on zinc oxide, which is used as a dielectric layer in window coatings and in [**R6**] to model the formation of layers of titanium on top of thin silver films. All these materials are used to make low-emissivity coatings on window glass.

3. References to the research (indicative maximum of six references)

[**R1**] Chalmers, C., Smith, R. and Archer, A.J., *Modelling the evaporation of nanoparticle suspensions from hereogeneous surfaces*, J. Phys. Condensed. Matter **29**, 295102 (2017), DOI: 10.1088/1361-648X/aa76fd

[**R2**] Chalmers, C., Smith, R. and Archer, A.J., *Dynamical density functional theory for the evaporation of droplets of nanoparticle suspension*, Langmuir **33**, 14490 (2017), DOI: 10.1021/acs.langmuir.7b03096

[**R3**] Areshi, M., Tseluiko, D., Archer, A.J., *Kinetic Monte Carlo and hydrodynamic modeling of droplet dynamics on surfaces, including evaporation and condensation*, Phys. Rev. Fluids **4**, 104006 (2019), DOI: 10.1103/PhysRevFluids.4.104006

[**R4**] Blackwell, S., Kenny, S.D., Smith, R. and Walls J.M., *Modeling evaporation, ion-beam assist, and magnetron sputtering of thin metal films over realistic time scales*, Phys. Rev. B **86**, 035416 (2012), DOI: 10.1103/PhysRevB.86.035416

[**R5**] Lloyd, A., Smith, R. and Kenny, S.D., *Growth of silver on zinc oxide via lattice and off lattice adaptive KMC*, J. Mater. Res. **33**, 847-856 (2018), DOI: 10.1557/jmr.2017.482

[**R6**] Zhou, Y, Lloyd, A, Smith, R and Kenny S *Modelling thin film growth of the Ag-Ti sy*stem Surface Science, 679 154-162 (2019), DOI: 10.1016/j.susc.2018.08.020

The quality of this research is recognised internationally in terms of originality, significance, and rigour. Papers [**R1**–**R6**] are published in leading academic journals in the area with rigorous peer-reviewed refereeing procedures. The research was supported by a £1.3m multi-university

EPSRC grant awarded to Prof. Smith (Title: “A multiscale modelling approach to engineering functional coatings” EP/C524322/1, 01/10/2005-30/09/2009).

4. Details of the impact (indicative maximum 750 words)

This impact case study describes the **economic benefits** of our research on two international companies. The first is **M-Solv Ltd**, which does research, design, engineering and manufacturing of micromachining and micro deposition equipment, specialising in bespoke, hybrid solutions. It has its main facility near Oxford and is part of the Hong Kong-based CN Innovations group, which has 11,000 employees engaged in the manufacturing of a wide range of products. The second company is **Asahi Glass Co**. (AGC), which is Japanese-owned and the largest glass manufacturing company in the world, operating in over 30 countries. Overall, **by guiding decisions, Loughborough Mathematical Modelling has brought economic benefit to two international companies.** We describe the four domains of economic impact below.

(a) Saved time and effort allocated to costly machine development work:

These days, inkjet printing is not just about transferring pictures and text onto paper. In manufacturing, inkjet printing is being used to create a variety of complex structures on surfaces. However, this is not without challenges. M-Solv Ltd wanted to tackle these issues in order to develop and make machines that use inkjet printing to manufacture the electrical connections required on touchscreens and solar-panels. By modelling the ink-drying process [**R1**–**R3**] we have been able to guide the process development. In particular, by modelling the process of the ink drying to form a connection from one metallic surface to another over an insulating surface, our models made clear predictions for how to reduce necking or even the breaking of the connections [**R1**]. In their letter of support [**S1**], Dr Adam Brunton, the Director of Business Development at M-Solv Ltd, reported that

> “[t]his research, together with the advice given to us by Prof. Archer since 2012 and still ongoing, has enabled us to optimise and improve our ink-jet printing manufacturing process, so that failures due to dewetting are eliminated. The advice and mathematical modelling saved us much time in the development process, by avoiding numerous trial and error experiments. <u>We estimate the staff time and materials cost saving to be £60,000.</u>”

Similarly, Dr Nicolas Rivolta from AGC Research and Development reported [**S2**] that the Loughborough fundamental work (2013-2020) [**R4**–**R6**]

> “has helped us guide experiments which saves us from carrying out costly experimental work… which might otherwise be of little practical value, thus saving staff time and costs. <u>The value to us of this is approximately £50,000 per annum</u>. It provides understanding to our in-house scientists and clarifies where we need to concentrate our research efforts”.

(b) Avoided negative financial outcomes:

AGC were considering using a thin blocker layer of titanium on top of the silver layer on their window glass coatings, to further improve the thermal properties. However, as stated in the letter of support [**S2**], the Loughborough “modelling investigated what happens at the silver-titanium interface as this bilayer was one of the materials we were considering as part of our multilayer coatings… [this showed] we would not be able to produce a sharp interface and therefore the amount of silver to be deposited would have to be increased”. AGC reported that this would have been costly and so in the end was not done **[S2].**

(c) Guided the planning of future production lines:

Loughborough researchers have modelled ways to deposit silver on window glass in order to create low-emissivity coatings, to reduce heat loss from buildings. Their proposed approach will significantly reduce the production cost and will be considered by AGC when their new production lines are installed. The AGC letter of support [**S2**], reported that “Loughborough have proposed a 2-stage silver deposition process... This would mean that less silver could be used to produce our low-E window glass, potentially saving the company several hundreds of thousands of euros per annum in addition to the ecological saving of non-renewable material.”

(d) Developed capacity and knowledge within M-Solv Ltd, to facilitate product development and enabling them to win substantial funding for innovation projects:

The Loughborough modelling work provided vital knowledge and insight to M-Solv Ltd which gave them the knowledge base foundation and confidence to continue to invest in developing their inkjet-printing based manufacturing technologies (known commercially as “One-Step Interconnect” and “One-Step Busbar”), which otherwise they might have abandoned. As a result of the expertise and equipment developed within the company, they were able to go on and win substantial innovation funding from Innovate UK and other EU funding. They write in their letter of support [**S1**]:

> “during the R&D process, the basic understanding gained from Prof. Archer’s work gave us the confidence to continue to invest time and effort in developing the technology. This enabled us to win Innovate UK funding eg project “One-Step Interconnect for Thin Film PV modules” (£1.2M) where we developed printing technology for solar panels and in which Loughborough University participated. We also participated in the significant, EU funded, collaborative R&D programme on perovskite PV, Espresso (€8M), led by IMEC, with many of the leading European academic and industrial groups as partners in which M-Solv received ~ €500k in funding. Thus, Prof. Archer’s group also helped us to develop our One-Step Interconnect and One-Step Busbar technology and equipment which will reduce capital expenditure, factory footprint and the unit cost of devices for our customers by approximately 10%. As a consequence, we are now entering the supply chain, with our manufacturing equipment being ready for sale to manufacturers of touch screens, smart windows and solar panels.”
>
> “We expect our tools to soon be using this enhanced inkjet printing technology in OEM factories worldwide, making devices for well-known phone and TV manufacturers. By end of 2020 first touch screen samples using, directly inkjet printed metallisation will be provided to customers and by 2022, sales of at least 5 of these new toolsets (~£1M each) are expected, making millions of screens per year.”

This shows that the Loughborough research and advice to M-Solv Ltd greatly broadened their knowledge and capacity, enabling them to develop new manufacturing equipment and processes, ready to work with the latest materials and technologies in, for example, touchscreen and solar panel manufacture. They conclude their letter of support [**S1**], by saying that

> “The past and ongoing collaboration with Loughborough University has significant impact on our business, providing much needed fundamental scientific underpinning for our manufacturing machine developments and has greatly broadened our capacity and knowledge.”

5. Sources to corroborate the impact (indicative maximum of 10 references)

[**S1**] Letter of support from M-Solv Ltd, dated 20th Nov. 2020.

[**S2**] Letter of support from Asahi Glass Co. (AGC), dated 21st Nov. 2019.