Cambridge
materialeyes

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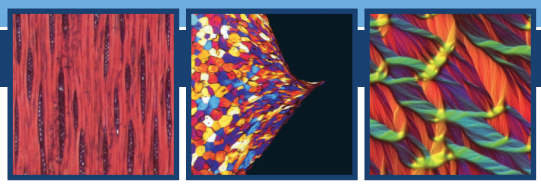
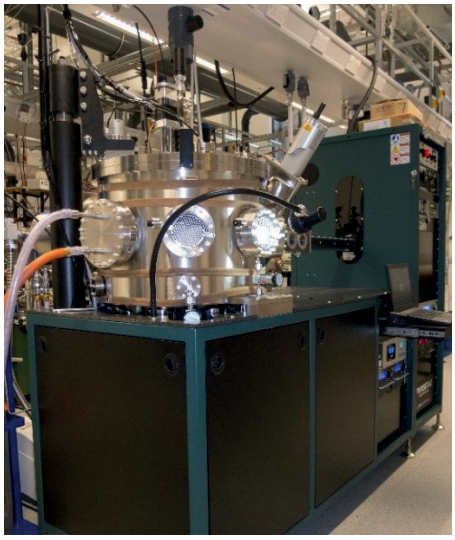


The Royce Institute @CAM

The Henry Royce Institute is a major investment by the EPSRC in materials research. The hub of the Institute is in the University of Manchester with partners in seven universities as well as the UKAEA and NNL. The Chair of the Institute, Baroness Brown and the Chief Scientist, Professor Phil Withers, were both members of staff in our Department some years ago. The Cambridge component is headed by Richard Friend (Cavendish) and overseen by the Maxwell Centre team, in which Lata Sahonta, previously a postdoc in Materials, is the contact for Royce facilities. The Cambridge work involves collaboration between five departments across the Physical Sciences and Technology and is focused on the "Materials for Energy Efficient Information and Communications Technology (ICT)" theme, one of the Institute's nine. The Cambridge funding primarily supports the acquisition of equipment. That, for our Department, includes wafer-scale atomic force microscopy (AFM), an automated sputter deposition system for complex heterostructures (pictured) and an associated focused ion beam (FIB) for device fabrication while Jason Robinson manages the Magnetic Property Measurement (SQUID) System housed in the Maxwell Centre.

The Cambridge work focuses on three important aspects of energy in ICT: generation, storage and efficient use. New materials capable of powering devices by capturing energy from the environment will be investigated, very much an interest in our Department (see, for example, *Issue 28*), with photovoltaic, thermoelectric, vibrational and electro-magnetic sources all being explored. We shall address the third component through magnetic, spintronic and superconducting systems. Our skills in making materials, especially on a nanoscale, and characterising their structure and properties will be vital. Work on energy storage will



primarily be carried out in the Department of Chemistry but we shall also be involved with the development of solid state batteries and with supercapacitors. Research using Royce equipment is not restricted to Royce themes: graduate students in some of the existing Centres for Doctoral Training (CDTs) in Cambridge will be taught to use Royce equipment and how to interpret their results and it is hoped that further CDTs in Royce areas will be established.

The Royce Institute is a national facility and so all of its equipment is available to researchers from industry and academia nationally, and booking systems and an appropriate nationwide scale of access charges are being set up, together with arrangements for training of users; indeed it is hoped that students in particular will experience more than one institution. We wish those involved in administering the Royce Institute locally and nationally all the best in their endeavours.

www.maxwell.cam.ac.uk/programmes/henry-royce-institute

Editorial

Welcome to the spring 2018 edition of Material Eyes. Much of the Department's attentions are now being focused on the (imminent) Strategic Research Review of the Department and the (still distant) Research Excellence Framework (REF2021). The former is almost the last of the reviews across Cambridge put in place after the last REF exercise and involves a substantial report on the Department's research activities, policies and strategy, and a two-day visit by the international review team in May. Although REF2021 appears a long way off, the University requires us to at least conduct a self-assessment exercise of our likely submission – presumably to identify potential problems well ahead of time.

We are assisted in both of these endeavours by the election of Manish Chhowalla as the next Goldsmiths' Professor of Materials Science. Manish is currently at Rutgers University in the USA where he leads a world-leading research programme on two-dimensional (2D) materials. Although 2D materials, such as MoS_2, WS_2 and $ReSe_2$ have been known for many years, and the first is an important dry lubricant, the isolation of graphene has focused attention on the electronic and chemical properties of a wide range of 2D materials. Already there is considerable activity on graphene in Cambridge but there is much less on the wider class of 2D materials and so this appointment strengthens the Cambridge presence in the area.

Professor Mark Blamire,
Head of Department

UNIVERSITY OF CAMBRIDGE
Department of Materials Science and Metallurgy

27 Charles Babbage Road
Cambridge CB3 0FS

msm.cam.ac.uk

Inside:

Materials Modelling

Exploiting modern computing power using a variety of scientific approaches to model the structure and properties of materials at all length scales, and indeed to predict novel structures, is an important and expanding part of the Department's research and teaching. A Materials Modelling course has been included in third year undergraduate teaching for over a decade and now there is a Materials Informatics course in the fourth. At graduate level, formal (inter-departmental) teaching is based in the Centre for Scientific Computing in the Maxwell Centre, and includes a Master's course in Scientific Computing leading to an MPhil degree and the EPSRC Centre for Doctoral Training (CDT) in Computational Methods for Materials Science (CMMS), now headed by James Elliott, that was described in *Issue 29*. The MPhil is primarily the responsibility of Nikos Nikiforakis in the Department of Physics while the CDT involves the Departments of Physics, Chemistry, Engineering and Chemical Engineering & Biotechnology as well as DMSM. In addition to starting their research, CDT students take the MPhil course in their first year. The existing CDT is jointly funded by the EPSRC and over 20 industrial partners for five cohorts of students, the last of which will start in October 2018. The EPSRC has recently closed a call for CDTs, and an outline application for renewal has been submitted.

The following examples, a sample of the total, give a feel for the range of modelling projects currently in progress in the Department. James Elliott is involved in the national Advanced Digital Design of Pharmaceutical Therapeutics (ADDoPT) project, a 4-year collaboration of pharmaceutical manufacturers, universities and other bodies. The aim is to make digital design of pharmaceuticals more widely accepted in the industry and thus to improve the development and manufacture of drugs. Lindsay Greer heads the European Research Council (ERC) "ExtendGlass" project in which molecular dynamics will be used to simulate changes in the structure of metallic glasses induced by "rejuvenation" (e.g. by thermal cycling) and to investigate crystallisation. Using different approaches Paul Bristowe and his colleagues include bulk materials and thin films in their investigations, not least with an emphasis on defects and grain boundaries, and correlation with experiment.

With the dramatic increases in available computing power in-house and in the University's Tier 2 High Performance Computing Centre, the expansion of modelling research has been very rapid since the new Department building was planned ten years ago, and the need for suitable space has become all too apparent. Modelling is not like experimental research: rather than working in a highly serviced laboratory, modellers need to work in a relatively undisturbed environment with opportunities to interact with one another. Some may spend all their time modelling but others will use modelling as just one component of a research project. A dedicated modelling area would form the permanent base for the former group while the latter group might work there for just a few weeks or months. No such area exists in the building at present, nor is there any spare space that could be restructured suitably. Following discussions with the original architects and an analysis of possibilities it has been concluded that the best option is to create a purpose-built "Computational Materials Centre" to provide up to 40 staff, students and visitors with working areas and a seminar room. It is proposed that the Centre will replace the present staff cycle shed on the south side of the building (pictured below – before and after). Discussions about funding – the cost is estimated to be about £1.7M – and timing are in progress. In Mark Blamire's words "The Materials Science building cost £55M to build and fit out in 2013.

This extension represents a small fraction of that total, but is key to developing our materials modelling activities and enabling them to take their place as one of the core capabilities of our world-leading department."

University Challenges

James Devine-Stoneman, who is researching superconducting spintronics in the Device Materials Group (an activity that has intrigued Twitter followers), is captaining the St John's College University Challenge team, which has now reached the semi-finals. The last stages will be broadcast in April. On his duties as Captain James comments, "The role of captain is that of a diplomat and decision-maker. On the bonuses, you confer and it's up to you to decide whose answer to put forward if there's a disagreement. The worst thing you can do here is to overrule a correct suggestion from a teammate – so usually I defer!"

Hearty congratulations to PhD student Tricia Smith (Medical Materials Group), who rowed at Bow in the victorious CUWBC boat on 24 March.

Jim Charles 1926 – 2017

Jim Charles joined the Department in 1960 and continued a close association after retirement in 1990. Throughout his career, he was resolutely a "Metallurgist", interested primarily in industrial processes, especially extraction and steel making, but his intuitive understanding of his subject led to important work in archaeometallurgy on the one hand and museum collections on the other. A full obituary will be posted on

www.msm.cam.ac.uk/news-and-events/news

A Memorial Service will be held at 12.00 noon on Saturday 26 May in the Chapel of St John's College to which members of the Department past and present will be most welcome.

ABC Forum 2017

Opening the 2017 Armourers and Brasiers' Forum, Bill Bonfield summarised the history of the Company and of the event and thanked the sponsors for the generous support that enables free attendance by participants from a wide variety of establishments in the UK and beyond. He also congratulated Serena Best, chair of the first session of the afternoon, on her very recent appointment as CBE.

In a wide-ranging survey of his current projects in materials processing particularly for healthcare, **Mohan Edirisinghe** (UCL), whose company AtoCap won the Venture Prize in 2010, described methods for creating very small particles, fibres and patches. Electrohydrodynamic, gyratory and microfluidic techniques, mostly operating at ambient temperature, have been developed, e.g. an electro hydrodynamic gun to deposit wound dressings and medical patches and microfluidic bubbling to generate tiny particles for subsequent coating with a drug.

Carbon is critical to the production of many important materials but it is commonly derived from fossil sources. **Magdalena Titirici** (QMUL) explained that one route to reducing use of such sources at the same time saving energy is to extract carbon from sustainable biomass derivatives using hydrothermal carbonisation. Typically, hydrothermal carbon (HTC) particles are about 200 nm in size and may have controllable amounts of porosity. A variety of potential uses including anodes in Na-ion batteries and even perhaps carbon dots were reported.

Ian Farnan (Cambridge) revealed that investigations of nuclear materials by NMR have produced important insights, although stringent safety precautions are essential especially for magic angle spinning of samples containing plutonium. NMR gives quantitative atomic scale information for specific elements, for example the proportions of atoms in crystalline and amorphous environments, an invaluable tool for studying the mechanisms and consequences of radiation damage and is leading to a revision of previous views.

After a brief introduction to the terminology of dielectric loss **Neil Alford** (Imperial) focused on combinations of materials and progressively smaller physical structures that show very low loss and so extremely high Q factors up to about 600,000. Several inorganic and (more surprisingly) organic materials have been successfully trialled in various geometries and MASER action, normally observed only at low temperatures, has been achieved at room temperature. The ultimate low-noise amplifier becomes a possibility.

Xun-Li Wang (City University, Hong Kong) then summarised the uses of elastic and inelastic neutron scattering in materials research, outlining several examples including the following. The depth of penetration by neutrons has revealed important features of friction-stir welding. Significant differences between the mechanisms of deformation in nickel as a function of grain size down to the nanocrystalline have been detected. A hitherto hidden amorphous phase in the supercooled liquid region of Pd-Ni-P metallic glasses has been discovered.

Introducing the presentation of the 10th annual Armourers and Brasiers' Venture Prize, Bill Bonfield reported that of the nine companies awarded Prizes so far seven are still operating. The Master, Mr Edward Pitt, then announced the award to Imperial College spin-out *Customem*, who have developed selective membrane cartridges to remove (often toxic) micro-pollutants from water which, furthermore, can be recycled.

Kelly Lecture

With the tantalising title "Bulletproof custard" **Mike Cates** (Cambridge) surveyed discontinuous shear thickening (DST) in very dense suspensions of hard particles in a liquid. Corn-starch in water provides easily made examples. The sudden onset of DST in industrial processes can have catastrophic effects. Experimental data have been acquired by various methods and computer simulation, treating the particles as microscopic ping-pong balls, has been helpful.

In Newtonian fluids the stress is linearly proportional to the strain rate but, as he demonstrated, there are many examples of non-Newtonian fluids. In DST the log(stress) versus log(strain rate) graph shows a sharp increase in slope with increased overall concentration of particles. Hysteresis is found when comparing the behaviour as a function of increasing strain rate from a low value with that for decreasing strain rate from a high value. This suggests that the graph should have an S-shape ("wiggle") in the vicinity of the instability. Batchelor proved that a suspension of hard particles in a liquid behaves either as a Newtonian fluid or, when the particles jam together, as a solid. What determines the jamming concentration of particles? Contact friction between the particles provides an attractive hypothesis but Stokes asserted that the particles never actually touch. If so, there can be no friction; there will always be lubrication. This was a simplification too far, not least because the particles are not perfect spheres. Building on ideas from Maxwell, Sam Edwards considered two sorts of contacts between particles, rolling and sliding and worked out the condition for rigidity and thus the concentration for jamming – but still no wiggle. Next a short-range repulsion between the particles can be introduced to put off the formation of contacts below some value of stress.

How does this help with the practical problem mentioned above when a liquid discontinuously thickens during processing? It confirms that the empirical observation that slippery molecules that can be absorbed on the surface of the particles are beneficial. The work has also shown that a high-frequency, low amplitude oscillating shear stress applied transversely to the direction of flow can significantly reduce the risk of thickening. In concluding, he noted that nothing workable as constitutive model has yet been found. Neither a linear model nor a quadratic one work so a full understanding remains work in progress.

In thanking Mike Cates for his excellent survey, Athene Donald commented on how widespread the phenomenon is and mentioned other important examples, including chocolate. Then Lindsay Greer thanked everyone who had contributed either as speakers or behind the scenes.

The next Forum will be held on 12 June 2018; **www.msm.cam.ac.uk/forum**

Andrew Moss – X-ray Vision

A wide variety of X-ray equipment is available in the Department, much of it highly specialised (e.g. high resolution diffraction for thin films, or small angle scattering), some of it providing for standard data acquisition from polycrystalline samples. All of it requires skilful care and attention to ensure reliable, consistent performance – mechanical, electrical and electronic. Responsibility for carrying out those demanding tasks or for summoning external assistance when necessary lies with Andrew Moss.

Andrew honed his skills as an apprentice at The Welding Institute, gaining valuable experience in handling vacuum equipment and earning a City & Guilds Certificate in Mech. Eng. In 1989, roundabout the time his family abruptly expanded with the arrival of triplets, he joined the Department to look after Tim Burstein's ESCA (Electron Spectroscopy for Chemical Analysis) machine in the basement of the Arup Building. Subsequently he took over the X-ray post in 1996 on Brian Seymour's retirement, so moving to a bigger basement – in the old Building alongside Pembroke Street. Then, in the summer of 2013 he oversaw the move of the X-ray equipment to his third (and altogether more spacious) basement – in the new Building. So, what is the greatest change he has noted in 20+ years of X-ray support? Computerisation has continued apace, of course, but arguably, the most significant change has been the introduction of reliable, high-resolution position sensitive detectors, accelerating data acquisition by about 10x. Well-maintained, useful equipment attracts users, currently some 60 or so of them, including some external users, so another of Andrew's jobs is to oversee the booking system. After that he's very happy to hand over these records to Accounts and to leave them to administer the charging system! With a regular influx of new users, training, including safety training, is essential and is mostly dealt with in collaboration with Mary Vickers.

Away from his busy basement much else keeps Andrew occupied. In *Issue 16*, it was reported that Andrew was then the General Secretary of ACUA, the Association of Cambridge University Assistants. With the passage of time and changes in the University's recognition of unions, ACUA merged with Amicus which was later absorbed by Unite. As a result, Andrew is now Chair of the CU branch of Unite and is a member of Unite's national Higher Education Industrial Sector Committee.

Recent changes have impinged on his life in more ways than X-ray detectors. Living in Oakington he is now able to commute to work through the huge new development at Eddington and to do so on an electric bike. For relaxation, he enjoys bowls – indoors in Chesterton and out-of-doors in Girton according to the season, and there is a fair-sized garden at home to maintain.

Congratulations

Serena Best, 2017 Hatfield Memorial Lecture

Stoyan Smoukov, Senior Lectureship, QMUL

Mario Amado, Assistant Professor, Salamanca University

Lewis Owen, Research Fellowship at Gonville and Caius College, Oct 2018

Ruth Cameron, President's Prize recognising a lifetime's contribution to the field, UK Society for Biomaterials.

Harry Bhadeshia, Adolf Martens Medal 2017, German Society for Heat Treatment and Materials and Honorary Fellowship, French Society of Metallurgy and Materials

Colin Humphreys, Henry Clifton Sorby Award, IMS (International Metallographic Society) and ASM International

Rachel Evans, 2018 RSC/SCI MacroGroup UK Young Researchers Medal

Angelo Di Bernardo, ESAS Prize for Young Researchers, EUCAS 2017 and 2017 Pippard Prize, IOP

Sioned Llewelyn, winner of a presentation prize, 2017 National Student Conference in Metallic Materials (Sheffield)

Amir Fakeeh, poster award at the Nanoenergy 2017

Editorial team: John Leake, Mark Blamire and Rachel Hobson **Comments to:** rjh24@cam.ac.uk

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