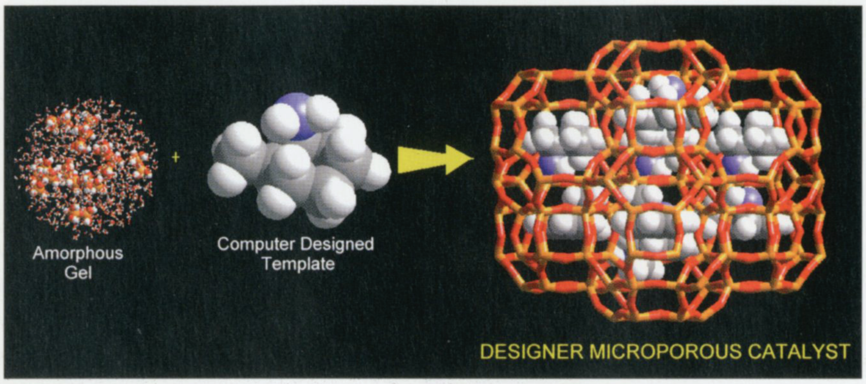
Cambridge material eyes

Spring 1998 Issue 5

A Pore Substitute?



Imagine a sieve so fine that it can be used to filter materials on a molecular level. Such things already exist, and oil refineries, washing powders and the pharmaceutical industry are all areas of application for these microporous materials known as zeolites. Dr Dewi Lewis explains "Zeolites do not have the close packed structures common to most crystalline materials: instead they have great holes in the middle (between 5 and 10 angstroms in size). Because these holes are of molecular size, these materials can be used both as 'sieves' on a molecular scale, and as highly selective catalysts".

There are approximately 108 known zeolites, many of which are naturally occurring, such as the semi precious stone, lapis lazuli. Because of their porous structure, about 98% of the crystal is accessible as surface, making them ideal for use as catalysts (e.g. for cracking oil) or as ion exchangers (such as used in washing powders).

"The important thing about zeolites is that the pores they contain can be made shape selective. To synthesise them, water is added to amorphous SiO_2 and a base. The cocktail is then heated under pressure and the solid crystallises. By adding organic bases as templates, the shape and size of the pores which form around the organic molecule, will hopefully bear some resemblance to it." Dewi Lewis, in conjunction with other researchers, is trying to understand this effect, so that zeolites can be designed for specific applications. A computer modelling technique he developed, known as ZEBEDDE (zeolites by evolutionary de novo design) grows molecules with a specific shape inside the pores. By using this program it is hoped that appropriate organic molecules to be used as shape templates can be designed from scratch, in a far more efficient and cost effective way than the current empirical approach.

Whereas oil refineries and washing powder manufacturers are interested in optimising existing materials, the pharmaceutical industries are searching for catalytic materials which will give them the high purity levels and high conversion rates that they are seeking. By synthesising zeolites with appropriately shaped pores, sieves and catalysts for purifying and synthesising drugs can be manufactured. ZEBEDDE will predict which organic molecules are appropriately shaped for a given application, and then it becomes a matter of making or finding such molecules.

http://www-img.msm.cam.ac.uk/D.W.Lewis/
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Editorial

Digital Definition

Our front page article focuses on one aspect of the burgeoning field of computational modelling. In it, Dewi Lewis describes his study of the role of zeolites (in effect, regular molecular-scale foams), in making the function of catalysts much more specific.

Computational modelling is influencing all areas of Materials Science and engineering. In fact, there is a modelling "hierarchy", much of it on the intermediate scale which is where the interests of many materials scientists fall.

Mesomodelling, as it is called, is one step up from the molecular scale and allows us to extrapolate to the macroscopic level where the qualities of new materials can be explored. So, just as modern engineering assemblies are designed almost completely by computer and, indeed, built and tested in digital space, we are doing the same thing with new materials to predict their properties and practical applications. Will this make those of us who enjoy more traditional laboratory pursuits redundant? Probably not, but the development of the "parallel" world of computational modelling is a major new facet of research and it is not surprising that it is changing the way we do Materials Science.

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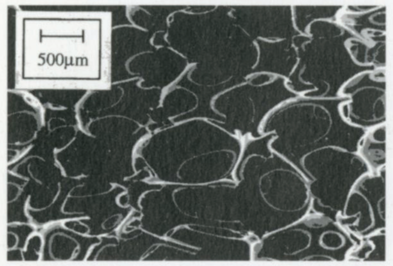
The hole story

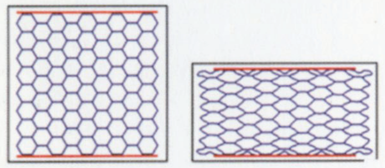
Polymer foams

Why is it that polymeric foams can be used in applications as diverse as cushions and cycle helmets? One reason is the range of different cell structures that can be produced and the way in which these affect material properties.



A scanning electron micrograph of an unstrained open cell poly-urethane foam.

This relationship is currently being modelled by Steve Thorpe, a student of Professor Alan Windle. The structure of such foams can be modelled as a network of elastic struts which are subjected to compressive strains.



Snapshots of a two dimensional foam model at zero and 40% compressive strain respectively.

By using an energy minimisation technique called 'simulated annealing', the deformation behaviour of these struts may be established. The computer algorithm used to achieve this is an example of Metropolis Monte Carlo methods, which were originally developed in the 1950s to investigate the equations of state for molecular systems.

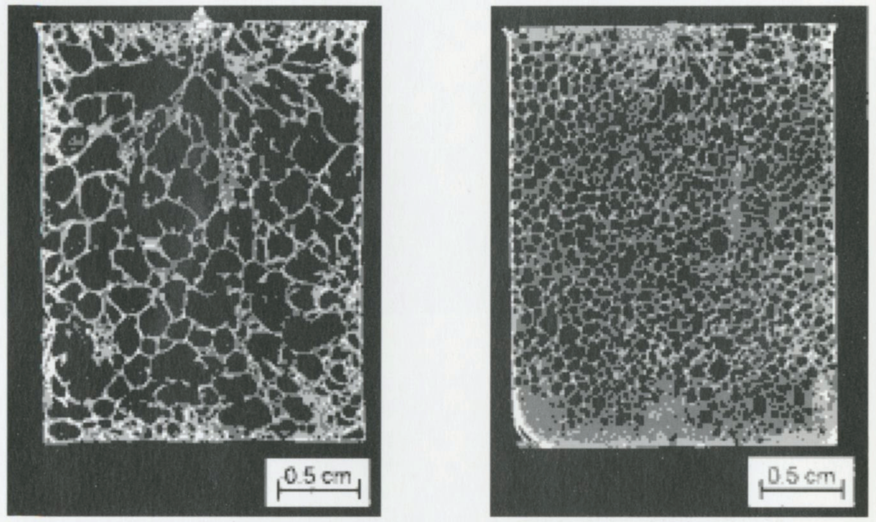
Through repeated application of strain steps, the stress-strain response can be determined and the resultant material properties predicted. In this way, the type of cell structure required to either absorb impact energy (as in a crash helmet) or to provide a great deal of linear elastic movement (as in cushioning), can be predicted.

Successful modelling will thus open the way for tailor-making polymeric materials according to their intended application.

Metallic foams

Processing routes for the production of foams are meanwhile being studied by members of Dr Bill Clyne's group, but in this case, the foams in question are metallic. Metallic foams have actually been around since the 1950s, but only recently has the technology of producing them been developed to the point where they are commercially available at competitive cost for bulk applications. Such metallic foams are generally manufactured from aluminium, to produce light weight materials that have excellent energy absorption and fire resistant properties.

Potential applications range from firewalls for the engine compartments of cars and blast proof doors for embassies to heat exchangers and aircraft wing sections. "There are lots of different ways of producing metallic foams," explains Bill Clyne. "If air is blown into molten metal on a conveyor belt, then the bubbles produced must be stabilised using ceramic particles.



Cross -sections through metallic foam materials showing the differences in cell structure that can be achieved by varying the processing route.

There can be problems in obtaining even pore sizes with this method, however.

Alternatively, powder routes can be used, where aluminium powder is mixed with a gas/generating powder such as titanium hydride, then blended and baked. The aluminium melts, reacts with the gas/generating powder and bubbles are formed. This method is often used to fill a mould, and produces foams with up to 90% porosity, but with a fully dense surface layer. A third route is where the gas generating agent is added to the melt and dispersed. This is attractive for producing large volumes at low cost and it need not involve the addition of ceramic to the cell walls, which adversely affects the material properties." This third route is being studied in Bill Clyne's group, the problem being how to disperse the gas forming powder uniformly within the melt before it reacts with the molten aluminium. This is being addressed by the use of coatings to delay the reaction. By suitable processing, different cell shapes, sizes and amounts of porosity can be produced. The work on metallic foams is being conducted by Vladimir Gergely from the Institute of Materials and Machine Mechanics in the Slovak Academy of Sciences, Bratislava, Slovakia where aluminium foams bearing the name 'Alulight' were developed.

How these factors affect the mechanical behaviour of metallic foams is also being modelled, both in the Department and in the newly set up Micromechanics centre, an interdisciplinary centre for computer modelling of materials, based in the Department of Engineering.

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PTP - enhancing links with industry

Glenn Parry a PTP associate

The production of scratch resistant coatings is just one of the topics being studied under a recent joint initiative between the Dept of Trade and Industry and the EPSRC to bring together Research and Technology organisations and Universities. Under the PTP scheme, (Post graduate Training Partnership) the University of Cambridge is linked with TWI to supervise students, (associates). There are currently 10 Associates, 7 in Materials Science, 2 in Engineering, and one in DAMTP (Dept. of Applied Mathamatics and Theoretical Physics). Topics range from the production of scratch resistant coatings to the characterisation of activated TIG welding.

Glenn Parry , a research student of Dr Ian Hutchings, is in the first year of his PTP project, "We are working on techniques to provide coatings for applications such as car windscreens which can potentially be anti-soiling as well as scratch resistant and hydrophobic." he explains. "Most people are familiar with scratch resistant coatings, as they are commonly used for sun glasses and spectacles. We can now produce more versatile coatings with superior properties as well as several functions, i.e. hardness and anti-oiling in a single coating." The coatings under investigation are ceramic/polymer composites (nano-composites) made using sol-gel techniques. The 'sol' is basically a colloidal dispersion of metal salts in aqueous solution. These are aged to grow an inorganic network and combined with a polymer to form a composite.

Before coming to Cambridge, Glenn completed his MPhil at Swansea University, working in conjunction with British Steel as part of a Teaching Company Scheme, another Initiative set up by the DTI. " It is good to see the different approaches to a problem, from an industrial and a university perspective," he comments. "By working in an industrial or commercial environment, students get experience of pressures associated with working in the 'real world'." Glenn , along with his fellow PTP Associates is expected to spend around 60% of this time at the Research and Technology organisation, and 40% at the Department. The exact balance of time is obviously dependent on the nature of the work being undertaken. For Glenn's project, he is lucky enough to have the use of a purpose -built sol-gel laboratory at TWI, and access to the latest equipment. "It would be very difficult for a university to provide me with this sort of facility " he comments.

Another advantage of the PTP scheme is that it gives the participating Associates access to a far wider group of colleagues than is normal for a PhD student. "I have the group in the Department, the PTP group, the people at TWI and the nation-wide group of PTP students who meet up on an annual basis to present the results of their work".

The first batch of students participating in this scheme were taken on in October 1996, and three further intakes are planned over the next three years.

For details of the PTP scheme, please contact Dr Rosie Ward, Academic Secretary at
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For more details about his work, contact Glenn Parry at
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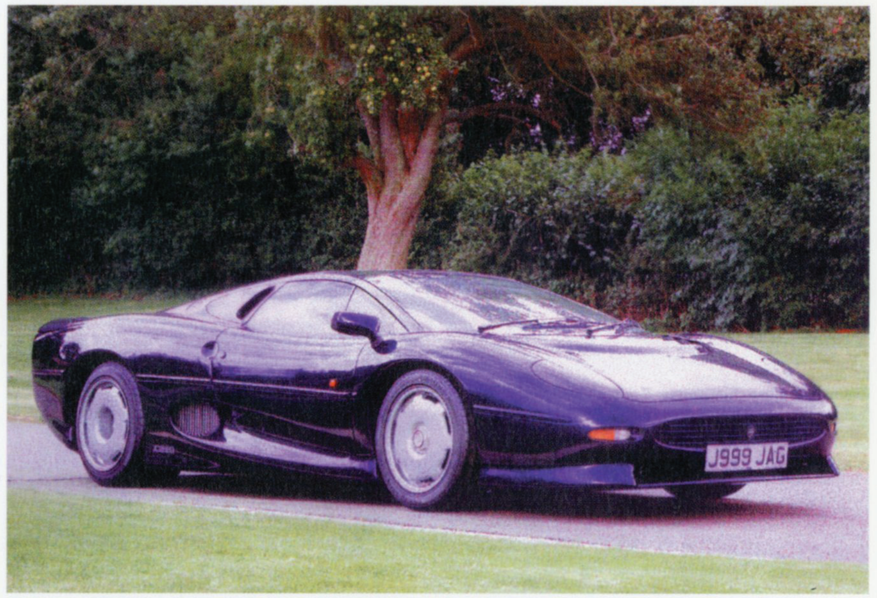
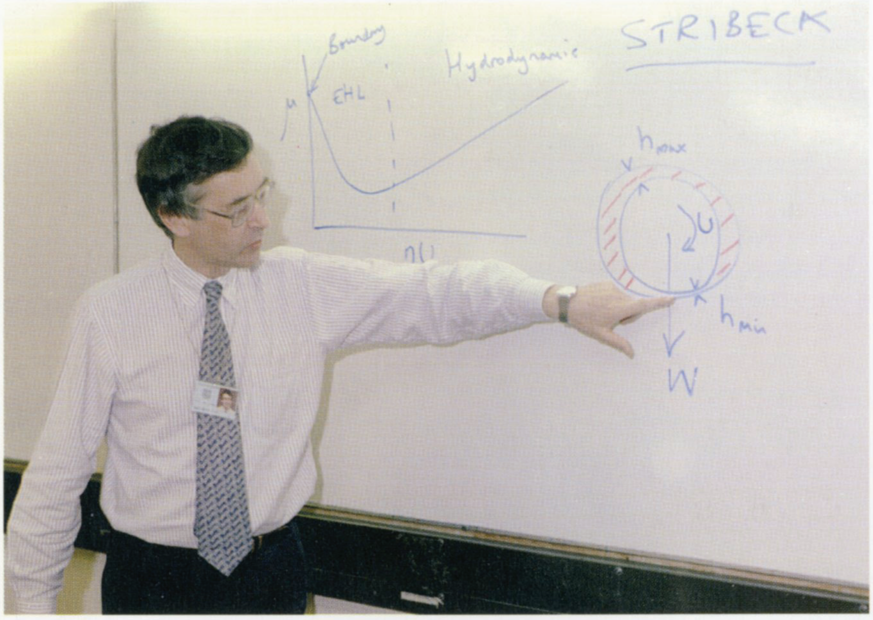


Scratch resistant coatings are being produced for applications such as car windscreens, and can be made to be hydrophobic for a self cleaning effect.

Department of Materials Science and Metallurgy

Friction in the Laboratory?

- a profile of Dr Ian Hutchings



Dr Ian Hutchings, who has just become the new Deputy Head of Department, is also Reader in Tribology: the study of friction, wear and lubrication. Having started his academic career in the Cavendish Laboratory, the University's Department of Physics, Ian made the transition to the Department of Metallurgy and Materials Science in 1977 as a Demonstrator. Until then he had naïvely assumed that materials science was 'simply' applied physics. "I was very quickly disabused of that idea," he remembers, when he found himself thrown in at the deep-end, supervising final-year students on the complexities of steel microstructures. He realised that he had not only a new language but a whole new subject to learn.

Ian was promoted to University Lecturer in 1982, and by that time he headed a flourishing research group studying many different aspects of the tribology of materials. He is the author of one of the standard texts on the subject 'Tribology: friction and wear of engineering materials', and runs an annual short course for industry on tribology as well as lecturing in the Department on the mechanical behaviour of materials, tribology, of course, and most recently, polymers. A couple of years ago, he was awarded a University Teaching Prize.

Looking back on his early days in the Department, Ian recalls how his research group had a laboratory right at the top of what is now called the Annexe. "All our computing was done on the early PET microcomputers with 32K memory - which cost £800 - and the programs had to be loaded from cassette tapes."

Of course the size of the Department has more than doubled in the last fifteen years, and that in itself has caused a number of problems, not the least of these being the lack of space. At the end of 1991, the Tribology group moved to the rooms they now occupy in the Austin building, the former home of part of the Cavendish Laboratory. Members of Ian's group work on a variety of topics, ranging from wear mechanisms associated with hard particles to the friction of paper, the wear of polymers in artificial knee joints (see Material Eyes, Autumn 1996) and damage to car paint caused by the impact of hard grit particles.

Besides his role in the Department, Ian Hutchings has considerable involvement with his college, St John's, where he was Tutor to engineering students for 13 years and is now the Chairman of St John's Innovation Centre, a science park on the northern outskirts of Cambridge.

When Ian became Deputy Head of the Department he took over the post from Dr John Leake who had filled that role for the previous six years. "Having a Deputy Head allows some of the responsibilities of the Head of Department to be delegated; the role can include simple jobs like signing grant application forms, but also more weighty issues such as Departmental strategy and finances."

Ian has four children, of which the oldest two are already at university themselves. "The undergraduates suddenly seem very young!" As for leisure time, he prefers to spend it away from humanity (except for his wife and children, of course) preferably gazing into infinity. Fortunately the fens are not a bad place for this pastime.

Congratulations to

- Dr. Bill Clegg on being awarded the Verulam Medal and Prize of the Institute of Materials for his outstanding contributions to the science and technology of ceramics and composites.

- Dr. Jeff Edington on his election to Honorary Fellow of Darwin College.

- Prof. Colin Humphreys on his appointment as the President of the Physics section of the British Association for the Advancement of Science for 1998/99.

- Dr. Ian Hutchings on his appointment as Editor-in-Chief of the journal 'Wear' from August 1998.

- Prof. A. Kelly who has been invited as the Yee Kuan Yew Distinguised Visitor to the Commonwealth of Singapore for 1998.

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