

SCIENCE WISE



Penny Sackett
on Stromlo & the
Giant Magellan Telescope

Making patterns with micro holes

Putting antimatter to work

Using X-rays to understand
crystals

ScienceWise is published by
the ANU College of Science.

We welcome your feedback.

For further information contact:

Christine Denny

T: +61 2 6125 5469

E: Christine.Denny@anu.edu.au

or

Jerry Skinner

T: +61 2 6125 3696

E: Jerry.Skinner@anu.edu.au

Cover image:

Professor Penny Sackett shares her
excitement on the Giant Magellan
Telescope (see story on page 3).

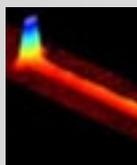
Photo by Tim Wetherell.

Views expressed in *ScienceWise*
are not necessarily the views of
The Australian National University.



Stromlo - a sense of possibility **3**

Penny Sackett explains why the Mt Stromlo Observatory is so well known around the world.



A double photon atomic laser **5**

Researchers from the Department of Physics have demonstrated how to make a laser a beam of atoms instead of photons.



Making micro patterns **6**

Chiara Neto has found a novel application for holes forming in thin unstable films.



Working with free radicals **7**

A new ARC Centre for Free Radical Chemistry and Biotechnology promises many advances for industry and health.



Chemistry in the superbowl **8**

Scientists at RSC are building host molecules that can carry other guest molecules to serve important functions.



New light on the dark side of matter **9**

The ARC Centre for Antimatter-Matter Studies promises to put antimatter on the map.



Shining light on diffuse diffraction **10**

Richard Welberry and how studying diffuse X-ray diffraction has changed over the years.

REPLICATING DNA

A team of scientists led by Professor Nick Dixon at the Research School of Chemistry has cracked one of the great DNA mysteries. In all cells, DNA is copied by a large molecular machine called the replisome. The replisome pulls apart the two DNA strands, and then it makes copies of both of the strands at the same time. In certain bacteria, a small protein called TUS binds to the last part of DNA to be copied in a way that stops the replisome when it faces in one direction, but not in the other.

"You can think of the strand separation part like a snowplough. The replisome tracks along one of the DNA strands and pushes the other one off it," Professor Dixon said.



Professor Dixon

The ANU team solved the important question of how TUS stops the replisome in this directional manner. "When the replisome comes along from one direction, separation of the two DNA strands simply knocks the TUS off as you'd expect," said Professor Dixon. But when it comes from the other direction, the strand separation near TUS leads to one of the DNA bases flipping over and inserting itself like a key in a lock in a perfectly shaped pocket on the surface of TUS. TUS is locked onto the DNA and this stops the replisome snowplough in its tracks."

Professor Dixon said the discovery, which was reported in the journal *Cell*, was important because TUS was found to lock onto the DNA very strongly and in an entirely new way. Strong interactions like this have great potential to be used in bio- and nanotechnology in fabricating new devices that might, for example, be used for early detection of diseases, Professor Dixon said.

More info: Nick.Dixon@anu.edu.au

THE RIGHT SCENT

A honeybee's ability to smell scent appears to be linked to the right side of its brain according to a new ANU study.

"Just as humans use different brain hemispheres for different tasks, it appears honeybees and other insects may also be right or left 'brained' for certain activities," PhD student Pinar Letzkus from the Research School of Biological Sciences said.

In the study, Ms Letzkus and colleagues found that honeybees use their right antenna to learn and recognise scent using three groups of bees in special smell learning exercises: one group had their left antenna covered, another group their right antenna covered, while the control group had neither antenna covered.



"The group with their left antenna covered – that is, the ones using their right antenna to pick up a scent added to sugar water – were just as competent at learning to recognise the scent as the control group, but the group with their right antenna covered were poorer at learning to recognise the smell of the sugar water.

"The results indicate that the right antenna in the honeybee is crucial in learning to recognise scent, suggesting that bees are right-brained when it comes to smell."

The study, published in *Current Biology*, is the first time that a right/left tendency for odour recognition has been shown in creatures such as insects. Ms Letzkus said the results could shed light on brain physiology and evolution more generally.

"But there is still much to be answered. One of the biggest questions is whether this system of left/right demarcation has evolved separately in insects and mammals, or whether it's a primitive system that for some reason has been genetically conserved in the evolutionary process."

SHAW PRIZE FOR ANU ASTRONOMER

ANU astronomer and Federation Fellow, Professor Brian Schmidt has been awarded the prestigious 2006 Shaw Prize for Astronomy jointly with US colleagues. Professor Schmidt, with Saul Perlmutter from the University of California Berkley and Adam Riess from the Space Telescope Science Institute, were commended for discovering the rate of the expansion of the Universe is accelerating. Their result requires the existence of a previously unknown 'force' connected to the fabric of space-time – known as 'dark energy' – that opposes gravity, driving the acceleration.

Professor Schmidt led an international team, including Riess, called the High-Z Supernovae Search that found the expansion of the Universe was speeding up, not slowing down (the commonly held view), by studying a class of exploding stars called Type 1a supernovae. Professor Perlmutter led a second team, which reached similar conclusions.

Professor Schmidt, from the Research School of Astronomy and Astrophysics, also leads the SkyMapper project, which will provide the first deep digital map of the southern sky, allowing astronomers to study everything from nearby objects such as asteroids in our Solar System to the most distant objects in the Universe called quasars.

The US\$1 million Shaw Prize is awarded in three categories – Astronomy, Life Science and Medicine, and Mathematical Sciences – to individuals whose work has resulted in a positive and profound impact on mankind.



Professor Schmidt

Stromlo – a sense of possibility

by David Salt

"If you were an astronomer in another country, you'd know the word Stromlo; you may not know the word Canberra, but, you'd definitely know Stromlo, and it would mean a whole host of things to you," says Professor Sackett, Director of the Research School of Astronomy and Astrophysics based at the Mount Stromlo Observatory.

And Professor Sackett is well placed to make such a statement having spent most of her time outside of Australia. She trained in theoretical physics in the United States and has served on a number of national and international astronomical advisory panels in the US and Europe.

"Historically the Mt Stromlo Observatory is known for the studies of the Sun, as well as for investigations on our closest galactic neighbours – the Large and Small Magellanic Clouds," says Professor Sackett. "It was also involved in the initial surveys of the southern sky that first probed for dark matter using gravitational micro-lensing back in the early 90s. More recently, its researchers have discovered some of the oldest known stars in the Milky Way and have discovered that the expansion of the Universe is accelerating due to the presence of dark energy.

"Stromlo has a strong attraction for researchers from around the world as a workplace to visit because of the interaction between engineers, astronomers and students – there's a sense of possibility here, and that's what it's best known for overseas. Another thing Stromlo is known for is producing quality graduate students. You'll find Stromlo alumni all around the world in positions of authority."

Professor Sackett took on the directorship in 2002, shortly before the wildfire of 2003. While the fire has changed much about the site, she believes the essence of Stromlo remained strong.

"At the end of 2002, we had just drafted a strategic plan for the school," comments Professor Sackett. "Following the fire, after we took care of our people, we began to ask 'what now?' And when we sat down and thought about it we realised that the strategic plan we had written didn't actually need much modification. In other words, our goals were the same, it was simply that the path we were

going to use to get there had now been altered. That was reassuring because it said that our core essence hadn't changed. And that essence was vested in our people, their reputations, their knowledge, and their ability to work together as a team.

"In many ways the fire brought the future forward, it made us answer questions that we might have otherwise deferred for years. So, for example, the fact that we'll be opening a new Instrumentation and Technology Building in the next few months is testament to us taking large steps forward, rather than small, incremental ones. We put a lot of thought into this facility and we're expecting it will be serving our needs for the next 40 years.

"When you come up the hill you'll see part of this new structure as you approach the observatory. You can't miss it, it's a large pale blue cube. That's the huge integration hall that gives us enough space and services to build the largest instruments for the next generation of telescopes, the telescopes that are being planned now but won't see first light until 10 years from now.

"The nature of what we do at Stromlo is definitely changing. The fire didn't cause this, but it has accelerated the change. The tendency has been to do more and more observing off the site at our Siding Spring Observatory. It's darker and better suited to this work. That's why the new Skymapper telescope we're building will be going there.

"Also, there are some sorts of observations that are not easily undertaken in Australia

and that's why we're strengthening our partnerships with international collaborations like the Giant Magellan Telescope. And to that end we're building capacity to create the components that will be used in the next generation telescopes.

"We had to decide if this was an area we

"There are only a few places on Earth where you can do this type of work. It's possible here because of the people"

wanted to continue. Interestingly, it was one of the things about which the staff was most in agreement. They thought that defining and creating the next set of tools for astronomy is something that sets us apart as an organisation. There are only a few places on Earth where you can do this type of work. It's possible here because of the people, because of the co-location of research astronomers, engineers and technologists of the highest levels. In many places you'll see these sorts of people separated from one another and that means that a lot of innovative ideas don't bubble to the surface. We can also work in a more efficient way because we're so close to one another.

"This is something special and something we want to build upon. Toward that end we've begun a program to involve graduate students in astro engineering and astro instrumentation. These skills are in very short supply the world over and students acquiring these capacities, quite frankly, can pretty much write their own ticket. Students entering this course are coming from a number of directions – engineering, physics and astronomy. They all bring different strengths and, while they're here, learn complementary skills."

Professor Sackett would like to see the strengths that make Stromlo such a special place today serve as a foundation for tomorrow's astronomers.

"I've said that our goal after the fire was to build the foundation to ensure that this place is as well regarded in 80 years time as it has been over the first 80 years," she says. "On staff right



"This is something special and something we want to build upon."

Setting sail with Magellan



Professor Sackett thinks the future of astronomy lies in projects like the Giant Magellan Telescope and believes Mt Stromlo has an important role to play.

now we have some extraordinarily well known and talented astronomers. In the years ahead I'd like to see the reins passed to another generation of astronomers that will pursue their own desires and strengths with the same vision and dedication. I'd like Stromlo to continue to develop and remain an attractive place that students from all over the world will aim for.

"In the coming years I expect we'll be putting out new results at a fairly high rate as the digital southern sky survey is completed using the Skymapper telescope. That instrument will see first light in the first half of 2007, though it will take a bit of time to complete the survey. I'm also hopeful that we'll be designing and building one of the instruments for the Giant Magellan Telescope, and that in 10 years time we'll be using that instrument in ways that we didn't even think possible today.

"Now that we're more visible following the fire, I'd also like to think that in the coming years the people of Canberra, and indeed Australia as a whole, will increasingly see Stromlo as theirs and as a source of pride. Just as for astronomers all around the world, I hope the mention of the word 'Stromlo' evokes a sense of achievement and possibility."

More info: www.mso.anu.edu.au

Australian astronomers, engineers, and technologists are part of an international partnership to design and build the world's most powerful telescope: The Giant Magellan Telescope. Scheduled for completion in 2016, it will be able to detect cosmic objects 75 times fainter than those seen with the Hubble Space Telescope, and produce images up to 10 times crisper. Using techniques currently being prototyped, this giant eye on the sky will become the platform for unprecedented discovery and insight into the evolution of planetary systems other than our own.

Professor Sackett will share her insights on the Giant Magellan Telescope speaking in Sydney during this year's National Science Week. She'll be talking about why the project is so special – and why it's so important that Australia be a partner in its development.

"There are many important themes connected to the Giant Magellan Telescope," says Professor Sackett. "One is that science, and in particular astronomy, is increasingly becoming an international pursuit. Projects like this enable Australia to engage with the rest of the world. Australia is very well placed in astronomy: our achievements are recognised all around the world. Space science is Australia's top-cited science, so it's starting from a very high position.

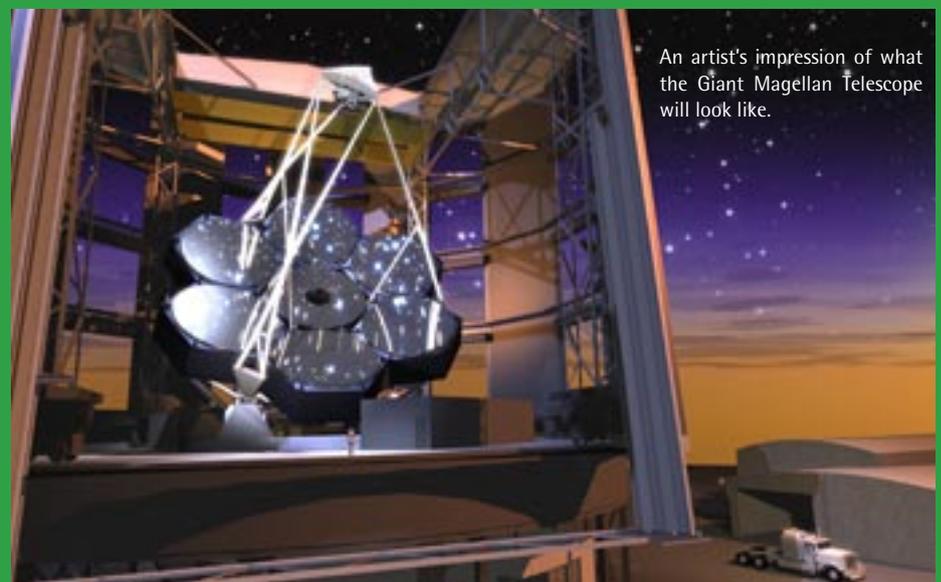
"In addition, a flagship project like the Giant Magellan Telescope, which will serve Australian science for decades, will inspire the next generation of scientists and engineers," an important consideration, says Sackett, given our increasing dependence on these disciplines as a culture. "It is gratifying to see that Australian industries are already planning

how they might be involved in this magnificent venture."

"We live in a special time for astronomy. These giant new telescopes will allow humans to study extra-solar worlds in greater detail than ever before, to ask questions about how they form, whether they exist in systems like our own or in completely different systems, and even to make some of the first measurements indicating the sort of atmospheres surrounding these other worlds. We're privileged to be participating in this historic exploration of the Universe.

"The technology that will be incorporated in this instrument, and what it will enable us to see, is amazing. If you think about all the news stories and all the gorgeous pictures and all the discoveries that have been made possible by the Hubble, then consider that Magellan will be many times more powerful. You can imagine how excited we are about observing with the Giant Magellan Telescope, and of course we're already writing down things we'd like to do with it when it comes on line. However, I would predict that the things that the telescope will be most famous for are things we haven't even thought of yet."

Currently ANU is the only non-US partner in the Giant Magellan Telescope, though Professor Sackett says, "Nothing would please me more than if our initial membership would prompt other institutions in Australia, or Australia as a nation, to join the partnership." The telescope, which will be sited in Chile, is now entering its detailed design phase which will take three to four years. Following that is the construction phase, which should take a further five years. More info: <http://www.gmto.org/>



An artist's impression of what the Giant Magellan Telescope will look like.

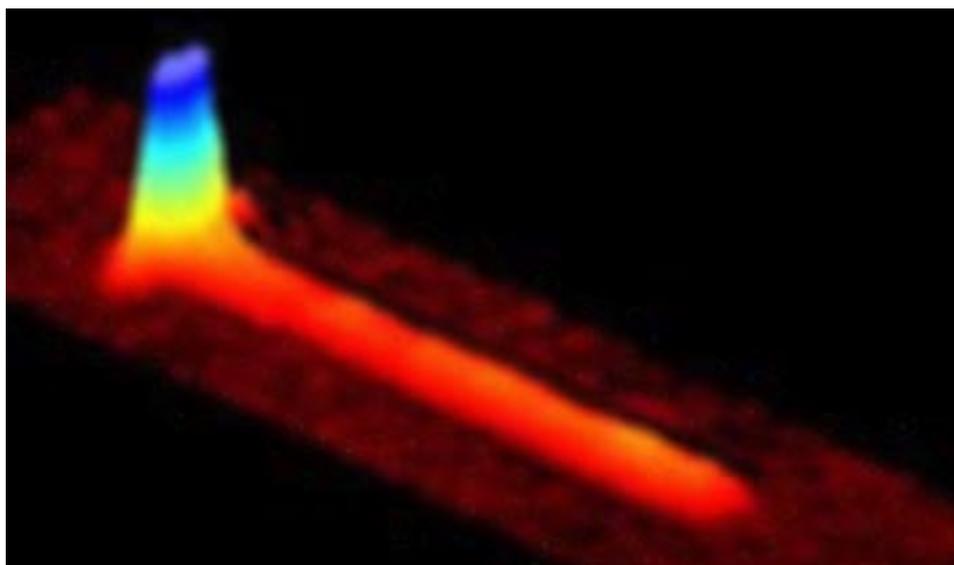
A double photon atomic laser

by Tim Wetherell

An optical laser beam consists of a stream of identical photons each with the exact same wavelength and phase. But the physics of lasers isn't restricted to photons; you can also make a laser from a stream of identical atoms. So-called atomic lasers begin with a super-cold cloud of atoms known as a Bose-Einstein Condensate or BEC. The atoms in a BEC are so cold that they take on an entirely new state of matter, each adopting identical quantum properties to the others, just like the individual photons in an optical laser.

In principle, by slowly releasing atoms from a BEC in a steady stream, it's possible to generate an atomic beam with all the coherence properties of an optical laser. As with so many things in science, the practice is a lot more difficult than the principle.

To achieve a BEC in the first place, scientists use optical lasers to slow or cool atoms to almost absolute zero. At such low temperatures the atoms become sensitive to the pull of magnetic fields and it becomes possible to trap them in a carefully designed magnetic cell. As the atoms cool further in the magnetic trap, they begin to condense into a BEC.



A beam of identical atoms, shown in red, pour out of a Bose-Einstein Condensate, shown in blue, to form an atomic laser. Atomic lasers may make a whole new generation of sensors possible.

This is a shadow image. To capture it the researchers fire a near resonant laser at the condensate and the atom laser beam. The atoms scatter photons out of the laser beam leaving a 'shadow' which is directly proportional to the local atomic density, just like sunlight shining through a cloud. This shadow is then imaged onto a CCD detector and what you see is simply the raw data from the experiment - a density map of the atom laser.

To release atoms from the BEC a radio frequency pulse is used to flip their Zeeman state, making them less sensitive to the magnetic trapping field and allowing them to tumble from the trap under gravity. However to make a really good bright atom laser, it's better if they all travel in a single direction with more enthusiasm than a mere tumble.

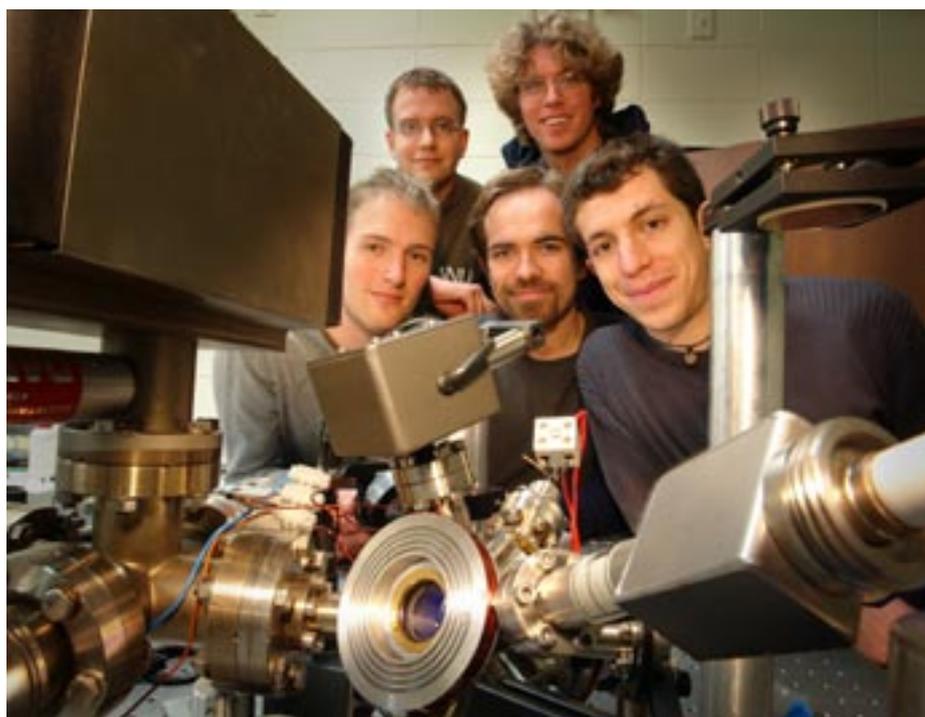
For almost a decade now theorists have been proposing a clever way of achieving atom

release from a BEC by using two photons of light to induce a double transition. With the angles, wavelengths and energy all just right, the effect is to flip an atom's Zeeman state thus freeing it from the trap, and also giving it a little kick using the momentum of one of the photons.

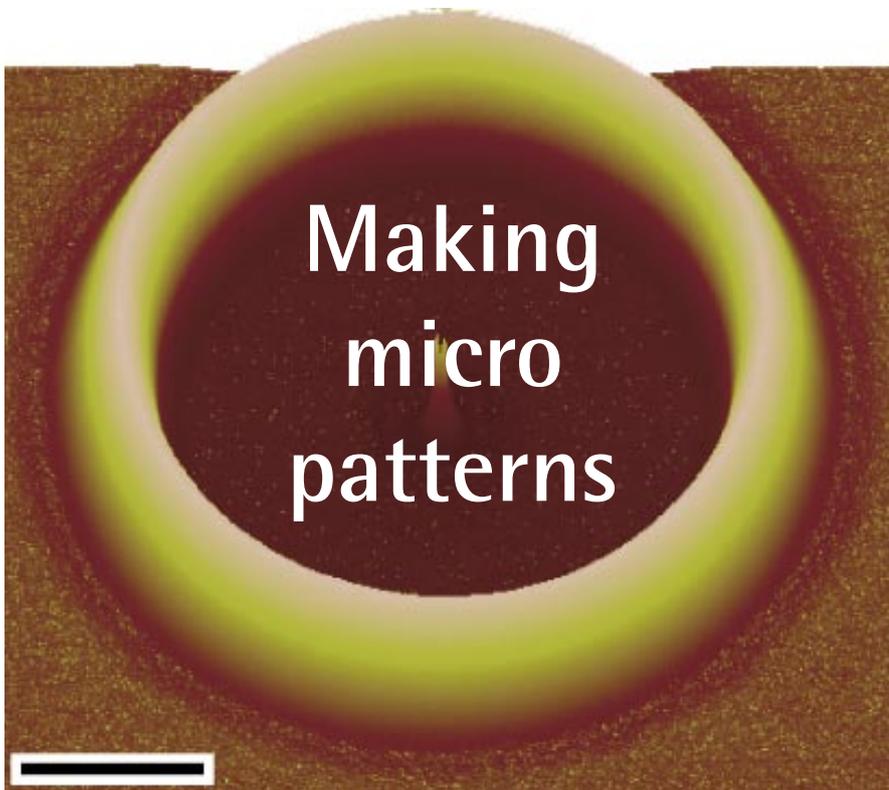
This is very complex to achieve in practice, and until recently had only been done using very short pulses to release little packets of atoms. However, scientists in the Department of Physics recently became the first group in the world to be able to utilise this double photon process to create a continuous steady release of atoms from a BEC forming a bright and highly coherent atomic laser. The work is one of the flagship projects of the ARC Centre of Excellence for Quantum-Atom Optics.

Because of their inherent physical properties, bright atomic lasers offer the potential to revolutionise many sensing applications. For example the theoretical limit to the accuracy of a rotation sensor using an atomic laser is 100,000,000,000 times as high as the same limit for an optical laser based system. Atomic beams also offer major improvements in time keeping which is vital to global positioning systems and to super quiet sensing used in gravity wave detection.

More info: Nick.Robins@anu.edu.au



The researchers behind the atomic laser. Clockwise from top right are Nick Robins, Julien Dugue, Paul Summers, Matt Jeppesen, and Oliver Topic.



Making micro patterns

by David Salt

It looks like a strange donut, but what's pictured here is actually a microscopic hole forming in a thin film of plastic (the length bar is 5 microns long). The film has been heated to become liquid and became unstable. It's then begun to break up. The process is known as dewetting and most people will have seen it happening when water on a glass surface breaks up into beads of water. The first step is for tiny holes to appear in the film of water.

This image was captured with an Atomic Force Microscope by Dr Chiara Neto, a physical chemist from the Department of Applied Maths, RSPSE. Dr Neto has spent considerable time researching this dewetting process. She's long wondered if there wasn't some application for which this process could be used.

"There's a lot of work published in this field about which films are stable, which aren't stable, and if they are unstable how they decay," says Dr Neto. However, it's all knowledge from a scientific point of view with little discussion on possible applications.

"Many times I would give talks on dewetting at different labs around the world and a typical question was: 'How might we use this information?' You can create these very interesting patterns in a controlled manner with different areas possessing different properties. Could this knowledge be applied to solve some problem?"

Dr Neto began investigating how a knowledge of the dewetting process might produce patterns with applications in other areas and quickly became aware of its potential for micro-patterning of biological substrates.

"It became apparent to me that it was possible to create micro patterns using dewetting that would serve a wide range of roles in biotechnology. However, unlike many of the existing techniques, Dewetting-Induced Biological Patterning – or DIBIP for short – is simple, versatile and cheap.

"A good way of understanding what it involves is by considering an example. Proteins readily adsorb to a film of the polymer polystyrene but not to poly methyl-methacrylate (PMMA). Suppose I want to create a pattern in which there are islands of protein-loving surface surrounded by a sea of protein-repelling surface. How might this be achieved? With a little knowledge of dewetting it's easy," says Dr Neto.

"First you coat a silicon wafer with polystyrene. This is done on a spin coater, a basic piece of lab equipment that costs a bit over a thousand dollars. It spins the wafer while you drop a solution of polystyrene dissolved in solvent on top of the wafer. As the solvent dries out this forms a nice even layer of solid polystyrene. Next, you build a layer of PMMA on top of the polystyrene.

"Then you heat the wafer with its bilayer of polymers till the polymers become liquid. The PMMA is more unstable and begins to dewet

or decay. Tiny holes begin opening up in the top layer revealing the underlying polystyrene layer. Because we understand the dewetting process we know how long it takes to form a certain number of holes of a certain size. We cool the bilayer when we've created the pattern we desire.

"We then expose the pattern to a protein solution and we end up with polystyrene islands covered in protein surrounded by PMMA which is protein free. With a few very easy steps this process has produced a patterned substrate that possesses micro-islands of adsorbed proteins separated by a protein-resistant matrix. The size and the distribution of these islands can be controlled simply by varying a few physical parameters, such as film thickness and dewetting time."

In principal, using different materials you can pattern any biological sample says Dr Neto. She's demonstrated that DIBIP works for protein and she's now working on devising a system for bacteria, in collaboration with Dr Rohan Baker from the John Curtin School of Medical Research. She believes she can also make it work for DNA, peptides, and other biological molecules.

While Dr Neto is confident DIBIP has enormous potential for biotechnology she also believes there's scope to push the technique into nano-patterning, with applications for nanosensors and application specific nanomaterials.

A provisional patent for the DIBIP method has been granted and Dr Neto is currently seeking suitable commercial partners for collaborative research and licensing in aid of market development.

More info: Chiara.Neto@anu.edu.au



Dr Chiara Neto with an Atomic Force Microscope, the instrument she uses to study the DIBIP patterns she creates.

Working with free radicals

by David Salt

What can you do with free radicals? We're not talking about free-spirited revolutionary anarchists, we mean free radicals in the sense of highly reactive chemical entities.

Free radicals are molecules with unpaired electrons that aggressively look for a mate so they're likely to take part in chemical reactions. Oxygen free radicals are particularly interactive as they react readily with many other molecules.

In the popular media you're most likely to read about free radicals in connection with your health. In the human body they can arise from fatty food, smoking, alcohol and a range of other nasties. They cause damage to our cells, convert good fats to bad fats and cause genetic damage. They're connected with the process of ageing, cancer and a range of disorders such as diabetes. Our best defence against such processes is the consumption of antioxidants that minimise free radical damage (indeed, most of the popular press on free radicals is connected to efforts to sell products containing antioxidants).

But this doesn't reflect the broader significance of free radical chemistry, because free radicals are everywhere and play central roles in an enormous range of industrial and biological processes. In addition to being agents of body damage, they also mediate a range of processes that keep us alive. White blood cells use free radicals to destroy bacteria and virus-infected cells. Other free radicals work in the liver to detoxify harmful chemicals. Free radicals are also a normal byproduct of everyday respiration and breathing. And radical chemistry plays a crucial role in many industrial processes.

"Free radicals are reactive intermediates, so we're talking about how and why reactions occur because when a chemical process occurs it's via reactive intermediates," says Professor Chris Easton, Deputy Dean of the Research School of Chemistry and Deputy Director of the new ARC Centre of Excellence for Free Radical Chemistry and Biotechnology. "So, if you understand free radical chemistry you can better control a wide range of reactions. Free radical chemistry plays an important part in many processes involved in the manufacturing

industry, the environment and human health.

"Australia has a rich history in free radical chemistry with a number of world-leading experts scattered among our universities and research institutions. Australian chemists were intimately involved in determining fundamental kinetic and thermodynamic parameters that revolutionised the field. Our scientists made crucial contributions to the synthetic chemistry of free radicals, as well as developing computational methods to accurately model radical energies. Australian chemists invented the Reversible Addition Fragmentation chain Transfer (RAFT) polymerisation process which has been critical to the development of a wide number of new polymer materials.

"Because of the enormous potential in free radical chemistry an ARC Centre of Excellence has been established to capitalise on Australia's existing strengths in this field. The centre, which kicked off in 2005 and will run for five years, has enabled some of our top free radical chemists to work more closely together in a unique research program that tackles issues that range from quantum chemistry through to chemical synthesis, biochemistry and pharmacology."

The Centre for Free Radical Chemistry and Biotechnology comprises researchers from ANU, the University of Melbourne (which hosts the headquarters of the new centre), the University of Sydney, Monash University and the Queensland University of Technology. Other participants include CSIRO, the Howard Florey Institute, Bluescope Steel, Dulux, Fosters Group and the Victorian Institute of Chemical Sciences.

"The diversity of the participants in the centre reflects the wide-ranging application of free radical chemistry," says Professor Easton. "So, for example, in the area of protective coatings on steel, free radical chemistry is allowing us to explore the possibility of chemically bonding a paint to the steel surface rather than just layering it on the surface as now occurs, which is the reason why they peel and crack. If you chemically bond the paint to the surface it's never going to peel and crack so the lifetime of the protective coat is going to be considerably extended.

"In the production of beer, radicals cause unwanted degradation. When beer sits for a



It looks like some radical work of art, and it is in a sense. This is the logo of the ARC Centre for Free Radical Chemistry and Biotechnology and the blobs represent the orbitals of the electrons of a carbon-centred radical.

while you get a beer haze forming which is associated with a bitter taste. That beer haze is a radical degradation process and so if you can stop that process you can stop the beer haze forming.

"In biotechnology, most diseases are about a biochemical process going out of control, many of which involve a free radical processes. If you can stop or intercept those radicals you can do something about it and come up with an essential treatment for a disease state.

"The work of the centre will have applications in all of these areas and many more," says Professor Easton.

"Here at ANU there are three groups based in the Research School of Chemistry involved in the centre's research: my group, Associate Professor Michael Sherburn's group and Dr Michelle Coote's group. Michelle Coote's group is in theoretical and polymer chemistry. Mick Sherburn's group works in synthetic chemistry and my group is working on the biological and radical chemistry interface. What sort of radicals are happening in biological systems or relevant to biological systems, and how can we understand and manipulate it in developing drugs.

"A particular interest is in peptide hormones. About half of the hormones in humans, animals and insects are peptide hormones, and the final step in their production is a radical process. We're interested in using fundamental free radical chemistry to develop new ways of regulating the production of these hormones."

So, Australia's fine tradition in radical chemistry looks set to continue.

More info: easton@rsc.anu.edu.au

Chemistry in the superbowl

by Tim Wetherell

Building molecules that can carry other molecules inside them has enormous potential in drug delivery and chemical catalysis. Scientists at the Research School of Chemistry have now built molecular host containers that they believe are good enough to be known as superbowls.

Back in 1987, Donald Cram, Jean-Marie Lehn and Charles Pedersen were awarded the Nobel Prize in chemistry for their pioneering chemical syntheses of molecules that mimic important biological processes. Cram's most significant work involved the development of the first fully encapsulating molecules, spherical molecules which were assembled by uniting two hemispheres. These 'host' spheres had the interesting property of being able to trap a small 'guest' molecule inside when the two halves came together. Since the sphere-trapped guest molecule is isolated from the surrounding medium, it exhibits different physical and chemical properties from the solid, liquid and gas phases. This observation led Cram to describe the interior of a host molecule as a new phase of matter.

Although brilliant in conception, these early sphere hosts were only able to hold small guest molecules of up to a dozen or so atoms. Further, once they were closed, by joining the two hemispheres, the hosts were difficult to open again so the trapped guest molecule was not available for use in chemical and biological processes. Associate Professor Mick Sherburn's group at the Research School of Chemistry has spent many years studying container molecules looking for better ways to overcome these twin problems.

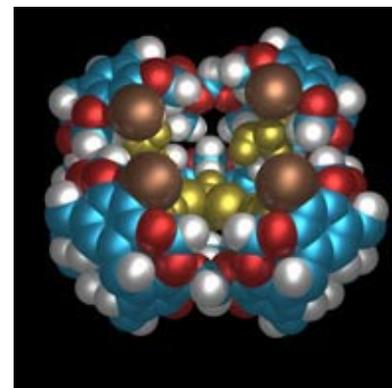
Recently, by combining six bowl shaped molecules, rather than just two, Sherburn and his group have been able to create a very large (on the molecular scale) spherical host molecule. The molecule is capable of containing much larger guest molecules, up to 100 atoms in size. The problem with release has been solved by removing one of the six bowls to leave five in the form of a vessel with a hole at one

end, rather like a microscopic jam jar, which Sherburn calls a 'superbowl'.

The stopper is formed by an ingenious set of smaller molecular groups which surround the hole and can, in effect, vary its aperture depending on their size and orientation. But unlike the familiar jam jars of everyday use, these microscopic molecular versions are quite particular about their contents. By slightly varying their internal structure, scientists are able to create sites that are attractive to some molecular groups while being repulsive to others. This opens up many exciting technological possibilities.

The larger internal volume of the ANU superbowl molecule is well suited to the scale of many important medicinal compounds such as the new cancer treatment Paclitaxel (Taxol). One of the problems with Taxol is its low solubility in water which makes delivery within the body problematic. The ANU researchers are hopeful that they will be able to engineer their superbowl so that it will hold a molecule of Taxol on the inside yet itself be highly soluble in water. Once at the required site, the door could be opened possibly using laser light or radio waves, and the Taxol could be released in high doses right where it's needed.

Superbowls also have potential applications in removing contaminants from the



A model of the superbowl holding five guest molecules (coloured gold).

environment such as the PCBs used in computer manufacture. Molecules similar to PCBs show a strong affinity for superbowl's hydrophobic interior but also can be readily removed from the host. These are the necessary attributes for separation technologies.

A third exciting possibility involves using superbowl host molecules to catalyse chemical reactions between small guest molecules. The ANU group has already shown that up to five different molecules are bound simultaneously in fixed locations inside the superbowl. They are looking at ways to chemically bond these guest molecules together and then release them to form products that would be difficult or impossible to create by other means. In this way, the superbowl acts like a microscopic molecular assembly plant.

More info: Michael.Sherburn@anu.edu.au



Members of Michael Sherburn's research group (from left to right) Alistair Longshaw, Laurence Kwan, Gomotsang Bojase-Moleta and Emma Pearson ponder the purple superbowl's possibilities. (Photo by Tim Wetherell)

New light on the dark side of matter

by David Salt

An ARC Centre of Excellence devoted to antimatter-matter studies has been established. Known as CAMS – the Centre for Antimatter-Matter Studies – it's hosted by ANU and includes other universities and government laboratories.

"Antimatter is the same as normal matter but with an opposite electrical charge," says Professor Stephen Buckman, Research Director of CAMS. "It's believed there's an antimatter equivalent for each of the known subatomic particles. The commonest form of antimatter used is the positron – the antimatter equivalent of the electron."

"If an antimatter particle comes in contact with a normal matter particle they annihilate and are converted into energy in the form of gamma rays. Antimatter is not easy to work with but there's a lot more to it than abstract physics," says Professor Buckman. "When antimatter meets normal matter it takes only a split second before it's gone but in that split second of interaction it's possible to learn a lot about the physical environment around the antimatter particle."

"And the gamma rays that are released are easily detected allowing researchers to pinpoint where the antimatter-matter particle pair was when it disappears. These aspects

of the interaction between antimatter and matter lend themselves to some very useful applications in the areas of medical scanning, materials characterisation and theoretical particle physics.

"There are two basic sources of antimatter on Earth: particle colliders and the radioactive decay of some isotopes. Antimatter used in diagnostic scanning and materials characterisation uses antimatter produced by radioactive isotopes."

One of the most common applications of positrons is in medical imaging and PET (Positron Emission Tomography) scans. The procedure involves injecting a patient with glucose containing a radioactive isotope which emits positrons. The body directs the glucose to areas of high metabolic activity, often indicating the presence of a tumour or immune system activity. The emitted positrons combine with electrons in the surrounding tissue, they annihilate and give off energy in the form of gamma rays. The gamma rays are easily detected and allow the source of the increased metabolic activity to be mapped, usually down to a resolution of 2-3mm.

"PET scans are a well-developed diagnostic tool and yet little is known about how positrons interact with biomolecules," says Professor Buckman. "One of the aims of CAMS is to study

the interaction of positrons with bio-molecules. In particular, we want to look at ways in which the efficiency of the process might be improved. We think we can improve the resolution of PET scans."

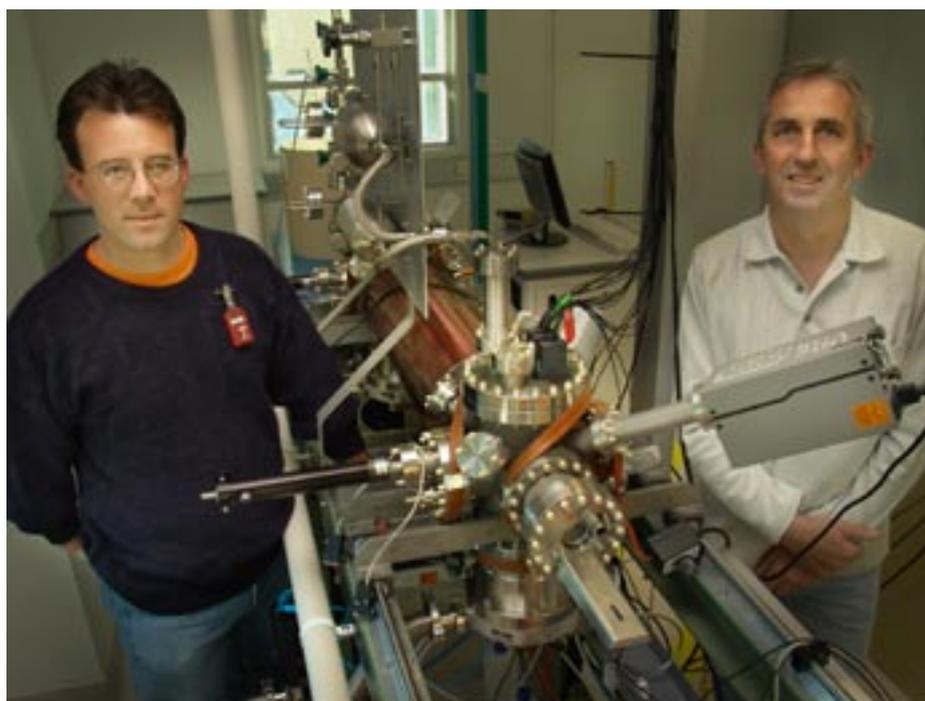
Positrons are also used in the analysis of materials. When positrons are fired into a material they tend to drift towards very small holes because they like to be away from the positive charge of the fixed nuclei in the material – like charges repel. When it finds a hole in the material, there are no electrons to annihilate with, so the size of the hole determines how long the positron lives.

"By looking at the lifetime of the positrons in the material, we can get information about the size and distribution of holes, or defects, that are as small as a nanometre in size," says Professor Buckman. "Holes of this size are related to important properties in some materials, such as porosity and conductivity. They can also be an early indicator of material degradation. In CAMS we plan to use one of the positron beamlines for the study of materials for various applications, from new generation plastics to silicon wafers."

The source of the positrons in the CAMS beamlines is a tiny speck of radioactive sodium 22. It's only a few nanograms in size, so tiny that you can't see it with the naked eye. The sodium sits in a lead-lined chamber at one end of the beamline. It emits around a billion positrons every second. After filtering and conditioning a small portion of these positrons are released in a tightly controlled beam for use in experimental research.

"This Australian facility will place us at the global forefront of positron physics," says Professor Buckman. "There is no other centre in the world with such an adventurous focus or such a breadth of activities involving positrons."

More info: www.positron.edu.au
or email Professor Buckman
<Stephen.Buckman@anu.edu.au>



Professor Stephen Buckman (right), Director of the Centre for Antimatter-matter Studies (CAMS) with Dr James Sullivan. The two scientists were responsible for the design and construction of the positron beamline. (Photo by Tim Wetherell)

Shining light on diffuse diffraction

by David Salt

Professor Richard Welberry has been working on methods to understand the arrangement of atoms and molecules in disordered crystals for many years. He's the head of the Disordered Materials Research Group at the Research School of Chemistry and his main tools of trade are X-rays and computers. The X-rays are used to probe the atomic structure of the material being studied. The computers are used to construct models based on the information from the X-ray studies.

This area of study is known as X-ray crystallography and it involves passing X-rays through the crystal lattice of the material being studied. The atoms in the lattice cause the X-rays to scatter, and by measuring the pattern of the emerging X-rays – the diffraction pattern – it's possible to calculate the arrangement of the atoms in the material.

In most types of crystallography you're calculating a model of an ideal crystal, a structure in which every unit cell of the lattice contains identical atoms in identical positions, which scatter beams to identical points in the diffraction pattern. These patterns are known as Bragg reflections (after the father and son team of W H and W L Bragg, who pioneered the science).

But real materials are never perfect. Individual atoms all deviate to some extent from their ideal positions in the average unit cell, and disorder within the crystal structure is often what gives a material its desirable properties. And this is where conventional X-ray crystallography has limitations because these variations from the ideal simply aren't picked up. To understand them you have to 'read between the lines' of the diffraction pattern, you need to interpret all the other information in the pattern. This is known as working with diffuse diffraction and it's where Professor Welberry and his team come into their own. Professor Welberry has been working on diffuse scattering for decades and believes a better understanding of diffuse scattering will greatly enhance our understanding of the relationships between nano-scaled structure and properties in a wide range of materials.

"Because it's difficult to collect and to interpret, only a few specialist groups around

the world practise the analysis of diffuse scattering," says Professor Welberry. "The vast majority of crystallographers neglect or simply don't notice the diffuse scattering that is always present in their experiments.

"My science is all about model building using diffuse diffraction," he says. "First, you observe things with real materials and X-rays, and then you try to build a model that will give the same diffraction pattern as the one observed.

"It's an iterative process. A model is set-up in terms of basic inter-atomic or inter-molecular interactions. Then you build a computer simulation of this model and calculate what diffraction pattern this model would produce. If that computer-generated diffraction pattern is the same as the observed X-ray diffraction pattern then you know you've created a valid model. However, if your computer model produces something different from the observed pattern then you need to go back and adjust your model."

Using this approach Professor Welberry's group has produced numerous insights on a wide range of materials including flexible organic molecules, advanced functional oxides and quasicrystals.

The task of calculating a diffraction pattern

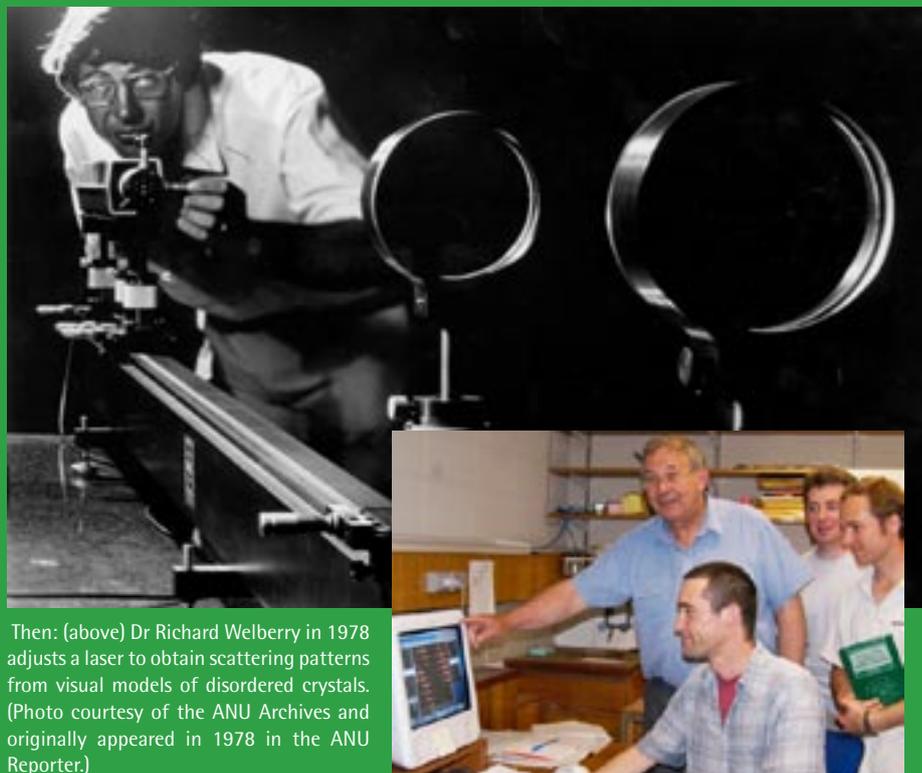
from a model is not to be underestimated. Indeed, it's so big that it was beyond the computing power of the available computers in the '80s.

"Before the early 90s, computers simply weren't powerful enough to create the diffraction patterns of the things I was interested in so I had to create them in another way," explains Professor Welberry. "I used to make models of atomic arrays in the computer and then create transparencies showing these models as a series of dots. I would then shine a laser light through these transparencies to project a diffraction pattern onto a screen or film in a camera.

"Fortunately, computers became more powerful and since about 1990 I could actually compute the diffraction pattern on the computer. However, the technique of creating diffraction patterns by optical projection has proved an excellent technique for teaching."

Professor Welberry's set of model slides are still used today in numerous laboratories around the world to explain to students the power and mystery of X-ray crystallography.

More info: Richard.Welberry@anu.edu.au



Then: (above) Dr Richard Welberry in 1978 adjusts a laser to obtain scattering patterns from visual models of disordered crystals. (Photo courtesy of the ANU Archives and originally appeared in 1978 in the ANU Reporter.)

Now: (right) It's all done with computers – both the building of the models and the calculation of the diffraction pattern produced by the models. Professor Welberry is pictured here with his research team (from left to right) are Mr Andrew Beasley, Dr Aidan Heerdegen and Dr Darren Goossens.



THE AUSTRALIAN NATIONAL UNIVERSITY

ScienceWise is published by
the ANU College of Science

Editor: David Salt

We welcome your feedback.

If you would like to be added to
our mailout or require further
information, please contact:

College Advancement Managers

Christine Denny

Christine.Denny@anu.edu.au

or

Jerry Skinner

Jerry.Skinner@anu.edu.au

ANU COLLEGE OF SCIENCE

T: +61 2 6125 5469

F: +61 2 6125 5190

E: CoS@anu.edu.au

<http://cos.anu.edu.au>

Views expressed in *ScienceWise*
are not necessarily the views of
The Australian National University.

CRICOS Provider No.00120C