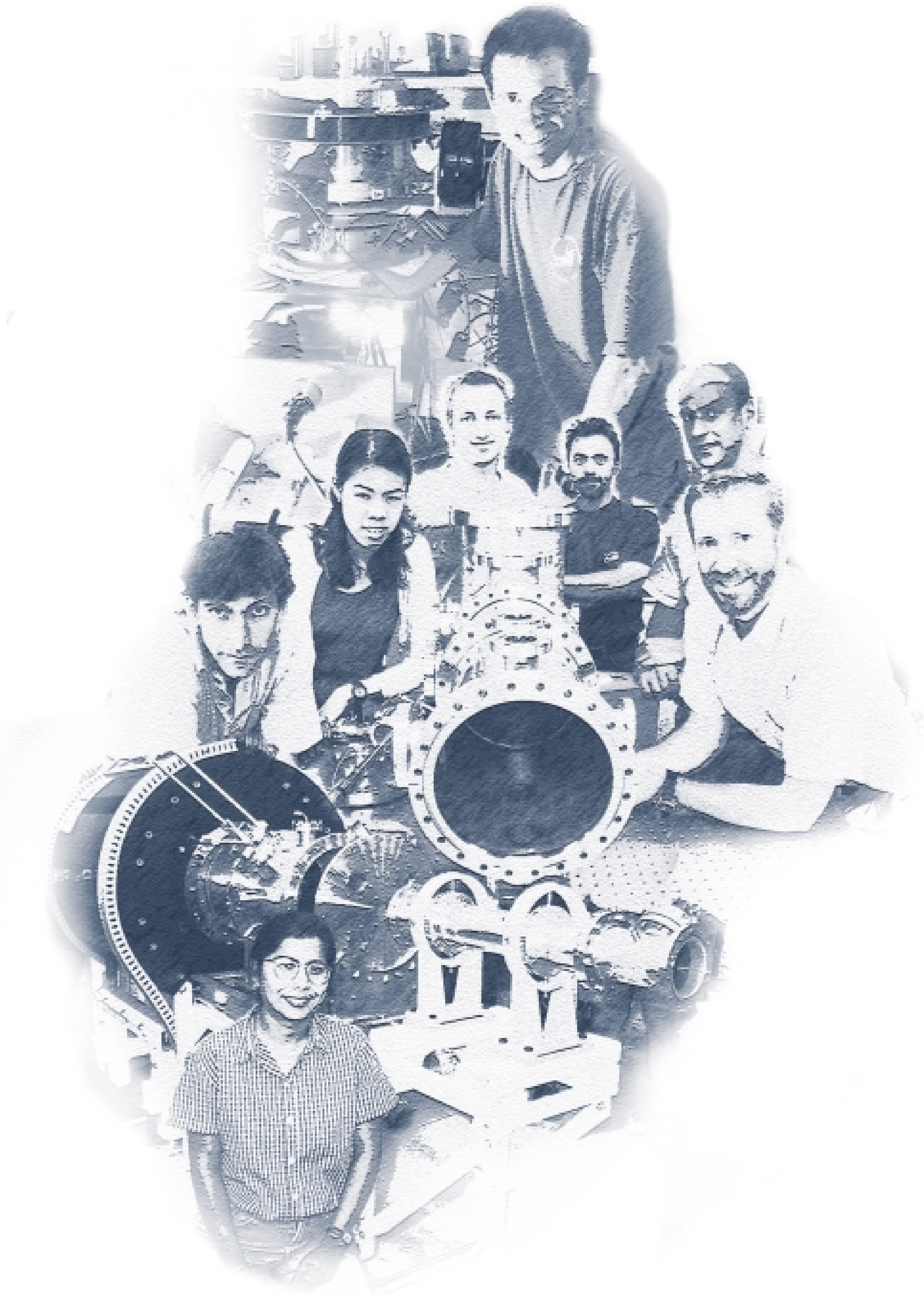
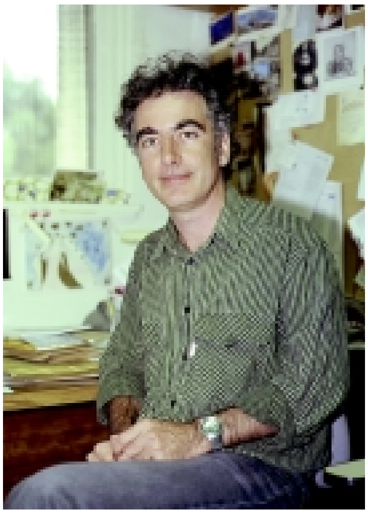
1 Research Accomplishments



Applied Mathematics



Professor Stephen Hyde
- Head of Applied Mathematics

The Department of Applied Mathematics performs research on fundamental and applied topics in colloid, surface and polymer science, largely in measurement of surface forces; on self-assembly of organic and inorganic structures at mesoscopic scales; and on disordered materials, mostly on micron-scale morphology and transport in porous structures.

Research Summary

2000 has been a very busy year for this Department. For this writer, (too) much of that business has been devoted to consolidation of research activities, to forward planning and to ensuring our long-term survival. Earlier in the year, we were reviewed by an international committee of the highest standing that resulted in a report of overwhelming confidence in the future of the department. The review process was strenuous and thorough, and we are justifiably proud of the result. We are very grateful for the committee for their rigorous independence and efforts during those hot days in February. We are now on a sounder long-term footing, and in the enviable position of recruiting the best talent we can find around the world in our perceived areas of strength: theoretical and experimental studies of complex condensed systems. Those systems range from surfaces and colloids to porous rocks. The work is at heart fundamental, but of direct interest to downstream scientists and technicians in the oil and cosmetics industries, the materials industries, and so on. Real advances have been made this year in characterisation of structure in disordered porous systems, using the armoury of integral and differential geometry, in understanding of a range of surface forces and in X-ray tomographic technology. It has been a busy year for research, with a record number of (mainly international) visitors, including physicists, biologists, geologists and chemists. We also hosted a two-week Workshop on Soft Condensed Matter that we hoped raised the awareness of this exciting inter-disciplinary area within Australia.

Research Accomplishments

Disordered Materials

Development of a X-ray micro-Computed Tomography Facility

The design and construction of a High-resolution X-ray Computed Tomography (CT) facility has commenced following the recent award of a RIEF grant to an University of NSW/ANU collaboration. Using a micro-focus X-ray source, a precision rotation stage and a scintillator coupled CCD array, the facility will provide us with a unique opportunity to examine complex three dimensional morphology in materials. The principal imaging modality will be cone-beam attenuation X-ray computed tomography, and the instrument will be capable of generating tomographs with up to 2048 voxels cubed and with voxel resolutions down to 2-3 microns cubed. One distinguishing feature of this facility will be the ability to study the flow of fluid through a porous network, or the shearing in granular material by performing time series experiments. *(B. Danaher, A. Sakellariou, T. Sawkins and T. Senden)*

Characterisation of Disordered Materials

We have quantified random morphologies obtained experimentally from an external micro-CT facility and for a range of disordered microstructural models utilising tools from integral, statistical and differential geometry and topology. We have investigated the effect of experimental distortion and noise on a number of quantitative measures. *(M. Knackstedt, C. Arns [UNSW] and K. Mecke [Wuppertal])*

We have generated the network model equivalents of numerous samples of sandstone obtained from the analysis of microtomographic images. We found that the description of the network topology is particularly crucial in accurately predicting multiphase flow

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properties. We are attempting to generate stochastic networks with topological properties representative of real sedimentary rocks. Accurate characterisation of the network topology requires the introduction of longer bonds. Measurements of pore geometry and correlations that occur at the pore scale in sedimentary rocks have also been made. (*V. Robins, A. Sheppard, R. Sok and M. Knackstedt)*

Development of Virtual Materials Lab

Worldwide, the petroleum industry spends in excess of a billion dollars annually on work related to the characterisation of reservoirs. A large part of this is spent on obtaining core material, performing tests and measurements on the core material and interpreting the test measurements in order to apply them to the field scale. Billion dollar field development decisions are made on the basis of these interpretations. A major uncertainty in the interpretations is the manner in which measurements on the core-scale relate to the field scale. Very little is known of the nature of heterogeneity on the core to pore scales. The interpretation and application of measurements on the core-scale to the field-scale is responsible for the introduction of major levels of uncertainty in field development decisions. A significant reduction in the level of uncertainty is the goal of this project. Collaboration with BHP and access to their store of core material and accompanying database of laboratory measurements will provide an opportunity to probe the role of heterogeneity in determining petrophysical properties. The project was successful in obtaining a SPIRT grant with BHP this year. *(A. Sheppard, R. Sok, M. Knackstedt; V. Pinczewski and J-Y. Lee [UNSW], L. Paterson [CSIRO Petroleum]; C. Balnaves and P. Behrenbruch [BHP Petroleum])*

Imaging materials via high-resolution X-ray CT and subsequent laboratory measurement of material properties will allow one to form a more accurate and comprehensive picture of the role of microstructure in governing the mechanical and transport properties of disordered materials. The longer-term aim is to offer researchers the ability to study a range of properties of complex materials in a virtual environment.

Simulations of the conductance, elastic and nuclear magnetic resonance (NMR) properties of a suite of Fontainebleau sandstone samples obtained from the analysis of microtomographic images was compared to experimental results. The agreement was excellent. The ability to develop accurate cross-property correlations is underway.

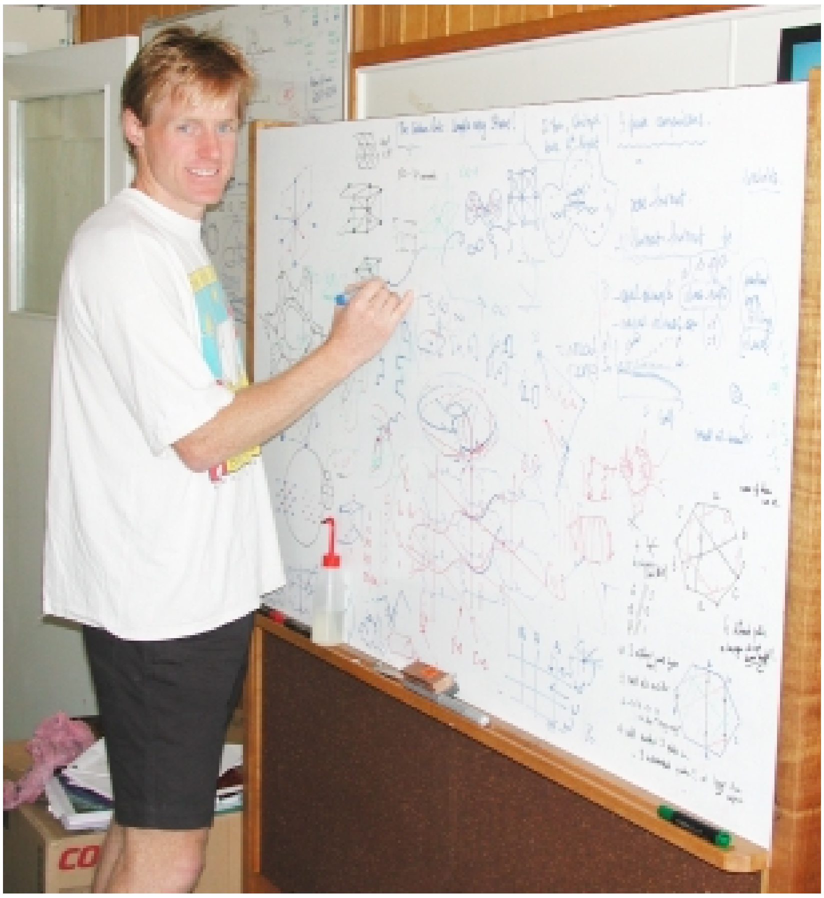
Fast computational modelling of multiphase flow has also led to the development of a virtual core-testing simulator which can accurately predict capillary pressure, relative permeability and residual oil saturations in core samples. In a first example, we have shown that experimental rate-controlled porosimetry results can only be quantitatively accounted for by incorporating correlated disorder. Current work has shown the importance of correlation on the prediction of residual oil saturation in sedimentary rocks.

These results have led to immediate international recognition and great interest from oil companies worldwide. *(M. Knackstedt, A. Sheppard; C. Arns and V. Pinczewski [UNSW])*

Droplet Penetration into Porous Networks: Role of Pore Morphology

The mechanisms of fluid penetration into porous media are investigated in etched porous networks. In particular, we investigated the role of pore morphology on droplet penetration and spreading rates, observed contact angle, and spatial distribution of fluid within the porous network. Experiments on a range of pore networks illustrated the critical role played by morphology in determining the physics of fluid penetration. A

Tim Sawkins and Tim Senden in the lead lined room that will house the new High-resolution X-ray Computed Tomography facility description of different imbibition events at the pore scale, and the time scale of the events is described. The consequences for imbibition into large disordered networks of capillaries are discussed. The strong effect of surfactant loading on fluid imbibition is noted. *(R. Roberts [Forestry], T. Senden, M. Knackstedt and M.B. Lyne [International Paper])*



Adrian Sheppard tackles some very hard sums

Mesoscale Physics

Novel Polycontinuous Mesostructures

Work continues on the enumeration and generation of novel morphologies as model mesostructures for complex fluids, including copolymers and lyotropic and thermotropic liquid crystalline systems. The surface geometry of partitions between novel multiple interwoven networks (derived from projections into 3D Euclidean space from the hyperbolic plane) have now been realised via generalisation of the Voronoi domain to these cases. The resulting partitions are fascinating hybrid structures, containing elements of bicontinuous, hexagonal and micellar morphologies, well-known in complex fluids. A number of novel partitions that carve space into 3D rod packings have also been deduced. These structures are being compared with experimental data collected on mikto-arm copolymers in Japan. *(J. Longdell, S. Hyde and H. Hasegawa [Kyoto University])*

Geometry of Strange Attractors

A numerical algorithm has been developed to probe the surface geometry of strange attractors. The code models the attractor as a surface, and estimates the curvatures of that surface. Results have been generated for the two best-known attractors: the Lorenz and Rössler cases. The long-term aim is to investigate whether 2D geometry and topology of attractors afford insights into the nature of the chaotic systems that lead to these attractors. A useful spin-off is the possibility to determine the differential geometry of other dynamic systems – be they intrinsically 2D or 3D – such as charge transport in solids. *(Y. Nagai [Kokushikan University] and S. Hyde)*

Bicontinuous Microemulsions

The possibility of a continuous structural evolution from bilayers to monolayers has been investigated in the didodecyldimethyl ammonium bromide – tetradecane – water microemulsion region of the ternary phase diagram. The signature of this transition is rapid "inflation" of length scales in the system on dilution, and small-angle X-ray scattering apparatus (SAXS) analyses allow us to check for this inflation. The SAXS data are consistent with this scenario, as are NMR data. This is a novel mesostructural transition that supports the notion of a continuity of geometries and topologies in lyotropic systems. *(M. Olla, M. Monduzzi [Cagliari University] and S. Hyde)*

Biomineralisation in Sea Urchins

Work continues on the ultrastructure of magnesian carbonate sea urchin skeletal plates. In particular, an apparent discrepancy between single-crystal optical behaviour and polycrystal X-ray diffraction behaviour is being investigated by X-ray diffraction, optical and electron micrography, and texture analysis of diffraction patterns. *(A. Christy, S. Hyde and F. Meldrum [Queen Mary and Westfield College, London])*

Novel Ultrastructured Inorganic Colloidal Aggregates Grown in Gels

Joint work with Granada continues on the formation of complex curved morphologies (typically at the µm scale) in carbonate crystallite aggregates grown in the presence of silica. There is now clear evidence of orientational ordering in these aggregates, with no long-range translational order between the crystallites. The materials are thus similar to (chiral) liquid crystals, though they are a complex composite of carbonate crystallites and silica. A local twist constraint between adjoining crystallites is sufficient to generate the most biogenic-looking aggregates (sheets and twisted ribbons). *(J-M. Garcia Ruiz [University of Granada], N. Welham, A. Christy and S. Hyde)*

Our Weissenberg X-ray camera has been rebuilt and used to collect diffraction data from helical barium carbonate aggregates grown in high-pH gels. A computer program written to calculate diffraction patterns from anisotropic crystal aggregates has been used to match the observed patterns, and it is evident that the helices show a high degree of preferred orientation. The full range of morphologies exhibited by these biomimetic aggregates is still being catalogued by field emission scanning electron microscopy of samples prepared in various ways, with a view to evolving a comprehensive model for the growth mechanism. *(A. Christy, S. Hyde, N. Welham and J.M. Garcia-Ruiz [University of Granada])*

Mesostructure in Poorly Crystalline Carbon

A naturally occurring glassy carbon ("shungite") is being studied, so far by field emission scanning electron microscopy, X-ray diffraction and transmission electron microscopy. It appears to consist of three distinct materials: an X-ray amorphous, extremely hard matrix phase, a silicate-carbon composite, and a material that is fibrous on the submicron scale. Investigation continues. *(A. Christy)*

Surface Physics

A Phase Transition of n-alkane Layers Adsorbed on Mica

Our previous studies of the films of n-octadecane and n-hexadecane adsorbed on mica surfaces have been extended to two other long-chain n-alkanes, n-tetradecane and n-heptadecane. Using data on the growth rate of capillary condensates between the mica surfaces in contact, and film thickness measurements, we have identified a transition in the structure of the adsorbed films a few degrees above T_m. As T decreases, the alkane layers appear to undergo a transition to a more ordered structure, akin to the postulated "surface freezing" of long-chain liquid n-alkanes. *(N. Maeda, M. Kohonen and H. Christenson)*

Surface Supercooling and Stability of n-alkane Films

The surface tension of n-octadecane was studied in the vicinity of the bulk melting point using both the maximum bubble pressure and Wilhelmy plate methods. The bubble surfaces were found to be supercooled below the surface freezing point. The onset of surface freezing is indicated by a sharp drop in surface tension at a constant temperature. This transition is accompanied by increased film stability resulting in longer bubble lifetimes at the liquid surface. Variations in bubble lifetime reflect changes in the interfacial mechanical properties of the film from liquid-like to solid-like. *(N. Maeda and V. Yaminsky)*

A Method for the Calibration of Force Microscopy Cantilevers via Hydrodynamic Drag

A new method for the *in situ* and non-destructive calibration of cantilevers used in force microscopy employing hydrodynamics is described. Using the notion that the viscous drag on objects is scale invariant for similar Reynolds numbers, the drag on a 500:1 scale model of a typical cantilever was compared with that of the actual cantilever drag within Stokes regime of laminar flow. The spring constant of the model cantilever was determined via static end loading with known masses, and the distributed load due to viscous drag carried out in neat glycerol. A master curve of the ratio of distributed to point load was determined as a function of distance from a horizontal surface. Similar curves were then obtained for actual cantilevers in water, the comparison of which to the master curve provided an estimate of the spring constant. (*N. Maeda and T. Senden)*

Thermodynamic Theory of Surface/Capillary Melting/ Crystallisation

General thermodynamic phenomenology of physical chemistry of interfaces (classical capillarity) explains and unifies new and old results on surface and capillary phase transition. The Gibbs adsorption equation provides the general thermodynamic framework for complete theory of these effects. To illustrate the fundamental principles we restrict our examples to simple single component systems. The results can be readily extended to cover more complex systems including surfactant solutions, Langmuir-Blodgett monolayers, liquid crystals and biological membranes. The associated notions are bulk phase transitions, homogeneous nucleation and crystal growth. *(V. Yaminsky)*

As an illustrative case we revisited the temperature dependence of the equilibrium size of t-butanol liquid capillary condensates, below the bulk freezing point, by means of the surface force apparatus. A simple capillary condensation interpretation is in good agreement with experimental measurements. *(Y. Qiao and V. Yaminsky)*

Adsorption from Solution at Solid – Vapor Interfaces

Molecular mechanisms of hydrophobic effects of cationic surfactants are explained by the surfactant adsorption at the silica (or mica) – water interface. We provided a retrospective comparison: radiolabel and contact angle results from the Paris group led by one of the authors several decades ago, and recent data that comes from our laboratories in Lund, Stockholm and Canberra on ellipsometric measurements of adsorption and wetting kinetics. The deposition mechanism of the static and dynamic de-wetting transitions is proved experimentally. A self-consistent theory based on these results explains equilibrium contact angles and contact angle hysteresis. *(V. Yaminsky, K. Eskilsson [University of Lund, Sweden] and L.T. Minassian-Saraga [Paris, France])*

A major Review of hydrophobic interactions has been completed. The issue has been shown to be nothing more than classical capillary condensation in one form or another and a unified and predictive accounting of the phenomenon was developed. *(B. Ninham, V. Yaminsky and S. Onishi)*

Characterisation and Direct Force Measurements of Fluorocarbon Monolayer Surfaces

We have prepared hydrophobic surfaces with heptadecafluoro-1,1,2,2,-tetrahydrodecyltriethoxysilane by LB method. The surface morphology, chemical composition, and the stability of the fluorocarbon surface thus prepared were examined with the atomic force microscope, X-ray photoelectron spectroscopy, and by contact angle measurements. The force measurements with the well-characterised surface were carried out with the interfacial gauge in dry air, humid air, and water. *(S. Ohnishi, V. Yaminsky and H. Christenson)*

Capacitance Dilatometry and Interfacial Friction in the Surface Force Apparatus

A capacitance dilatometry attachment has been installed on the Surface Force Apparatus. The distance between the active surfaces is obtained from the capacitance of a cylindrical parallel plate capacitor measured with a variable ratio transformer bridge, the surface separation is made to vary with a magnetic force transducer. The method permits measurements of forces between opaque surfaces over periods of time ranging in suitable circumstances from tens of milliseconds to days. The attachment is able to measure adhesion of single crystal mica surfaces with high accuracy and reproducibility, and has been used to measure forces between mica surfaces in electrolyte using the droplet method. Measurements have been made of the dispersion force between mica surfaces in air. It was found that above 20 nm separation, the Casimir-Polder theory that takes account of retardation fits the results much better than the van der Waals theory. *(A. Stewart)*

Measurements have also been made of the interfacial friction between single crystal mica surfaces using the friction attachment for the Surface Force Apparatus that has recently been constructed in the department. In contrast to ordinary friction which involves shear and fracture of asperities in the contacting surfaces, interfacial friction occurs without observable damage between the atomically smooth surfaces. A previously unreported peak has been detected in the interfacial friction of mica in a dry environment after the surfaces have been separated for only a few seconds and then brought together again. *(A. Stewart, S. Ohnishi and H. Christenson)*

Theory of Atomic Forces and Intermolecular Interactions

With the use of the generalised multipolar gauge, a completely general proof is obtained for a result asserted by J.H. Van Vleck in 1932 but never fully proved by him. Specifically it is demonstrated that the matrix elements of the magnetic moment operator are independent of the origin of the vector potential for electromagnetic fields that are non-uniform in space and non-constant in time. Also using the multipolar gauge, a simple and exact conversion of the interaction Hamiltonian of radiation with matter from the form A.p to E.r plus higher order terms is demonstrated. *(A. Stewart)*

Formation of Vesicular Tubes from the Extension of Fused Phospholipid Bilayers

The molecular details of adhesion mechanics in phospholipid bilayers have been studied using Atomic Force Microscopy (AFM). Under tension, fused bilayers of dipalmitoylphosphatidylcholine yield to give non-distance dependent and discrete force plateaux of 45.4, 81.6 and 113 ± 3.5 pN. This behaviour may persist over distances as great as 400 nm and suggests the stable formation of a cylindrical vesicle which bridges the bilayers on the two surfaces. The stability of this connective structure may have implications for the formation of pili, the sexual apparatus of bacterial conjugation. Sexual reproduction in bacteria is an important phenomenon in the evolution of bacteria and its detailed study is essential to many aspects of medicine, genetic engineering and public health. *(J-M. di Meglio [Université Louis Pasteur and Institut Universitaire de France], N. Maeda and T. Senden)*

Flow of Thin Liquid Films

We have used the Surface Force Apparatus to measure the rate of growth of liquid capillary bridges between two surfaces in contact. For liquids with low vapour pressure, the rate of growth of the capillary bridge is determined primarily by flow of thin adsorbed films on the surfaces. Our measurements can thus be used to obtain information about the flow properties of very thin liquid films (thickness 1-10 nm), a problem of interest in numerous practical applications. *(M. Kohonen and N. Maeda)*

Capillary Condensation of Water between Silica Surfaces

Numerous studies of the capillary condensation of water in glass pores have reported deviations from the Kelvin equation. However, these studies are limited by the presence of leachable ionic components of the glass. We have now studied the capillary condensation of water between pure amorphous silica surfaces. The measured mean radii of curvature of the condensates are in agreement with the predictions of the Kelvin equation. *(M. Kohonen and D. Antelmi [RSC])*

Adsorption Kinetics of Cationic Surfactants to the Silica-Water Interface

Studies of the adsorption of cetyltrimethylammonium bromide to the silica-water interface have been extended. A second cationic surfactant CPBr has been investigated. Reflectometry studies have been supported by Atomic Force Microscope Images revealing that surface aggregates are formed below the Critical Micelle Concentration (CMC). These aggregates are slow to form and the requirement that monomers pack into aggregate structures is the cause of the Slow Adsorption Regime. Above the CMC aggregates adsorb rapidly and directly to the silica-water interface. *(V. Craig, R. Atkin and S. Biggs [Chemistry, University of Newcastle])*

Dynamic Measurement Using an Atomic Force Microscope

The hydrodynamic drainage force that is developed when a sphere approaches a wall perpendicularly is measured. It was found that the no-slip boundary condition is not applicable for high viscosities and high shear rates. The degree of slip at the boundary is quantified by the slip length. The relationship between surface properties, solution properties and slip-length has been investigated. *(V. Craig, D. Williams and C. Neto)*

A modified commercial AFM that permits rheological properties to be measured concurrently with the surface interaction forces has been applied to the measurement of surface forces. The phase and amplitude information provide extensive new information on the behaviour of complex systems such as the interaction between two surfaces bearing adsorbed polymers. *(V. Craig, S. Notley and S. Biggs [Chemistry, University of Newcastle])*

Observation of Conformational Changes of DNA Under Different Ionic Strength and Types of Ion by using Atomic Force Microscopy

The aim of our work is to use atomic AFM, for studying the type II restriction endonuclease EcoRI cleavage of DNA and its dependence on background electrolyte, ion pair and buffer.

Plasmid DNA was studied in aqueous solution. AFM imaging was performed in tapping mode AFM in air on mica. Images of plasmid DNA adsorbed from water show a mixture of super coiled and relaxed forms and only a few plasmids left on mica without any ions were seen. By adding 4 mM $MgCl_2$ the plasmids became more condensed on the mica implying that the plasmids had compacted into a super coil. The density of plasmids on mica was significantly higher than in pure water. Divalent cations, such as $MgCl_2$, form a bridge between the negatively charged phosphate backbone of DNA and the negatively charged surface of mica. By reducing the concentration of $MgCl_2$ to 1 mM, repeated scans of plasmid DNA gave an image of the entire molecules with a good signal-to-noise ratio and most of the plasmids were entangled or super coiled. By changing the anion of 1 mM magnesium chloride (Cl) to acetate (OAc), the plasmid in most cases appeared as short bent lumpy molecules, and a few were coiled or entangled, even though the plasmid density was the same as with chloride as anion. *(H-K. Kim [Chalmers University of Technology, Sweden], V. Craig and B. Ninham)*

Bulk Chemical Physics

Interaction of Surfaces or Macromolecules in Aqueous Solvent

A few years ago, in calculations of double layer structures and interactions we started using potentials of mean forces between ions as evaluated in recently published simulation studies with molecular aqueous solvent. On the basis of the exact generalised McMillan-Mayer theory of solutions, we can now follow and improve approximations at each successive stage. The theory also shows that short-range solvent interaction resulting from packing of molecules is almost perfectly additive regarding to the electrostatic part of the force. It led us to a new development where effective potentials are obtained from simulation results on correlations using analytical integral equation methods, rather than the reverse Monte Carlo simulation pioneered by the Stockholm group.

In new work we included the interaction of ions adsorbed onto the surfaces and found oscillatory behaviour, very similar to measurements of forces performed in this department 15 years ago and not understood until now. Our accuracy is gradually improving, and we expect quantitatively accurate results and reasonable predictive power in the next year or two. *(S. Marcelja)*

Shapes and Deformation of Surfactant Vesicles

When surfactants are mixed in water, small bags or "vesicles" can form. These have applications in the cosmetic and pharmaceutical industries. For vesicles composed of one kind of surfactant the shapes which form have been much studied and are now reasonably well understood. The same cannot be said for vesicles composed of two or more surfactants. We have been studying such systems, starting with two-dimensional vesicles. A number of interesting morphologies occur, such as mushroom and peanut shapes. These morphologies are controlled by the spontaneous curvatures and the relative amounts of each surfactant. *(I. Miller and D. Williams)*

We have started work on the elastic properties of vesicles. Our work involves the study of vesicle deformation by various forces such as an attractive potential wall, or compression between two plates. This work has applications to experiments using micropipettes, optical tweezers, or the atomic force microscope. We approached these problems using a combination of simulation and approximate theoretical models. *(I. Cooke and D. Williams)*

Toroidal Condensates of DNA

When DNA is placed in the presence of a condensing agent or "glue" it collapses to form toroids. Our previous work has focussed on why this occurs. We have recently completed a study of how the hexagonal packing of the chains affects the toroidal structure. This packing induces a series of sharp transitions in the winding number and major radius of the torus as a function of chain length. Winding numbers corresponding to closed shells are strongly favoured and winding numbers corresponding to a spare loop are forbidden. The potential landscape as a function of winding number consists of a series of minima separated by barriers. In some cases these barriers may be high enough to produce long-lived non-equilibrium tori. *(G. Pereira and D. Williams)*

Mechanisms of Enzyme Activity as Revealed by Coion and Buffer Dependence of Restriction Enzyme Activity

The source of the activation energy that allows cutting of DNA by restriction enzymes is unclear. A systematic study of cutting efficiency of the type II restriction endonuclease *Eco*RI with varying background electrolyte ion pair, and buffer reported here, shows only a modest dependence of efficiency on cation type. Surprisingly, efficiency does depend strongly on the presumed indifferent anion of the background salt. What emerges is that

Nobuo Maeda ('Nobby') receives the Director's Award for the best student research paper competition between the background salt anion and the buffer anion for the enzyme and DNA surfaces is crucial. The results are quite unexpected and counterintuitive from the point of view of conventional theories. However, taken together with recent developments in surface chemistry the results do fall into place, and also suggest a novel mechanism for enzyme activity as an alternative to metal-activated hydrolysis. Microscopic cavitation in a hydrophobic pocket might be the source of activation energy.

This work together with parallel work on effects of dissolved gas on colloid stability and intermolecular interactions (*M. Alfridsson, B.W. Ninham and S. Wall [Chalmers University*]), and work in progress with Professor Piero Baglioni (University of Florence), on coion binding to micelles with nucleoside headgroups) confirms the predictions of Professor Barry Ninham and Dr Vasilli Yaminski. The foundations of colloid science embodied in the classical DLVO (*Derjaguin, Landau, Verwey, Overbeek*) theory, theories of interfacial free energies, and extensions of the Debye Huckel theory of solutions are fundamentally flawed. These do not deal with all important specific ion-Hofmeister effects. They are further deficient insofar as they treat dispersion interactions in a linear theory, separate dispersion interactions from electrostatic interactions, and ignore dissolved gas entirely. *(B. Ninham; H-K. Kim; E. Tuite and B. Norden [Chalmers University of Technology])*

Surface Tension of Aqueous Ionic Solutions

The simplest solution, and the most important from a biological viewpoint, is that of salts in water. In most cases these are strong electrolytes, i.e. fully dissociated. It is a remarkable fact that the change of interfacial tension of a system as simple as salt in water, remains unexplained. We are currently working on a theory of these systems including specific ions effects. *(M. Bostrom, B. Ninham and D. Williams)*

Growth Mechanism of Single Wall Carbon Nanotubes (SWNT) Produced by Laser in the Presence of Transitional Metal Catalyst

A thorough analysis of experimental results allowed us to derive a self-consistent model for the interpretation of the formation of SWNT's by a continuous wave (CW) CO_2 laser in an Argon-filled chamber, and we proposed a set of new experiments for further clarification of the nanotubes' growth mechanism. For nanotubes formed in a gas phase and in the presence of transition metal catalyst, the aim of these experiments is to reveal the dependence of the nanotubes' parameters on Argon pressure in the experimental chamber, and on the temperature in the nanotubes' formation zone. In the first set of experiments we used a CW CO_2 laser with fixed parameters as a target evaporation source and changed the Argon pressure in the chamber between 200 and 500 torr. Another set of experiments studied the dependence of the nanotube parameters on the temperature in the formation zone. The control of temperature in the evaporation area is performed by an additional Nd:YAG laser with variable parameters, while the initial heating and evaporation of the target is carried out by the CW CO_2 laser with fixed parameters. (*E. Gamaly; A.V. Rode; W. Maser, E. Mu-oz, A.M. Benito, M.T. Martinez and G.F. de la Fuente [Instituto de Carboquimica, CSIC, Spain])*

Participants of the Soft Condensed Matter Workshop

The Applied Maths buildings in the spring time

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Barry Ninham, MSc WA, PhD Maryland, DTech (hon causa) KTH Stockholm, FAA

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Andrew Stewart, MA ScD Cambridge, AM Harvard, EE Col, DIC PhD London, FAIP, FIE
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Andy Christy, MA PhD Cambridge
Vince Craig, BSc PhD (ARC Fellowship) (from July)
Satomi Ohnishi, BSc SUT, Tokyo, PhD Saitama, Japan
Tim Senden, BSc PhD (ARC Fellowship) (from March)
Adrian Sheppard, BSc Adel PhD (from July)

Adjunct Fellows
Mark Knackstedt, BSc Columbia, PhD Rice (jointly with School Pet. Eng., UNSW) (ARC QEII Fellowship)
Rob Sok, BSc PhD Groningen
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Vanessa Robins, BSc, MS PhD Colorado
Arthur Sakellariou, BSc Melbourne
Tim Senden, BSc PhD (ARC Fellowship) (until March)
Adrian Sheppard, BSc Adel PhD (until July)

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Stuart Ramsden, GradDip Film & Television Swinburne

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Jean-Marc di Meglio, PhD Paris VI
Eugene Gamaly, PhD DSc Moscow (Professor)
Bruce Hyde, BSc Bristol, PhD DSc (Professor)
Hye-Kyung Kim, MSc Yeungnam University (until June)
Wieslaw Kaczmarek, MSc PhD Poznan
Brent Lindquist, BSc Manitoba, PhD Cornell
Hiroshi Maeda, DSc Kyushu (Professor)
Siewert-Jan Marrink, School of Pet. Eng. UNSW
Klaus Mecke, DipPhys PhD München
Fiona Meldrum, MA Cambridge, PhD Bath (June-September)
Yoshinori Nagai, DSc Waseda, Japan (Professor)
Christophe Oguey, PhD, Ecole Polytechnique Federale (Lausanne)
Kevin Osborn, MB, BSc, DRACR
James Quirk, AO, DSc FTS, FAA, WA (Professor)
Ewa Radlinska, MSc Warsaw, PhD
Staffan Wall, BSc PhD Göteborg
Nicholas Welham, B.Eng Leeds, PhD Imperial College

Senior Technical Officers
Jack Derlacki (until July)
Anthony Hyde, AssocIE Aust
Tim Sawkins

Departmental Administrator
Diane Wallace (part-time)

Atomic & Molecular Physics Laboratories

Dr Brenton Lewis - Acting Head of Atomic & Molecular Physics Laboratories

http://wwwrsphysse.anu.edu.au/ampl

"Low energy atomic and molecular interactions lie at the heart of many everyday phenomena and devices. For this reason, atomic and molecular physics is both a fundamental and enabling science. Staff of these Laboratories pursue a broad spectrum of experimental and theoretical research into the properties and interactions of atoms, molecules and solids."

Research Summary

Atomic and molecular physics is a pervasive branch of science as its understanding underpins almost all low energy chemical reactions, many of which are of fundamental importance to our environment and to the technological devices and applications that play such an important part in modern life. The Atomic and Molecular Physics Laboratories are engaged in a broad range of experimental and theoretical studies of the interaction of electrons and photons with atoms, molecules and solids, in order to both further our understanding of the fundamental processes, and to provide information that is critical to an understanding of the applications.

As has been remarked upon in previous reports, in recent years there have been substantial changes in the staffing of the Department and in the profile of our research activities, enabled by considerable success in obtaining external funding. While this year has represented primarily a period of consolidation and exploitation of these new activities, we have also continued our external-funding successes. In particular, we have achieved new recurrent strategic funding for a Solar-Terrestrial Environmental Program (STEP) of research from the Institute Planning Committee of the ANU, which will lead to two new appointments in the Department (one jointly with CRES). In addition, we were successful, in a joint RIEF proposal with the University of Western Australia, in obtaining considerable funding for the construction of a National Facility for Electron Spin-Correlations and Spintronics.

It remains a significant challenge to staff to construct new apparatus adequately without the aid of external funding. The new STEP appointments will help in this respect, but we face a number of increasing pressures. First, the replacement of valuable staff who leave. This year, Dr Maarten Hoogerland and Kevin Lonsdale move to new pastures; we thank them for their sterling service. Second, the difficulty in attracting quality staff, given the existing exchange-rate problems. For example, this year we lost the IAS Fellow, won last year through the ANU's strategic competition, to a six-figure US$ salary. Third, the new ARC system will provide further challenges, principally the need to replace fixed-term positions with ARC appointments. We feel confident that we will do well under the new system, however. Finally, the long-standing problem of attracting graduate students from a diminishing pool remains. Only the Department's Atomic Manipulation activity boasts an adequate student cohort. We are redoubling our efforts to attract further students and remain committed to providing a first-rate supervisory and research environment. This year, two students have graduated (Weijan Lu and Agus Purwanto).

Finally, recognition of the quality of research performed in the Department is evident from the number of personal awards and distinctions achieved by its members during 2000. Professor John Carver was awarded the 2000 COSPAR International Cooperation Medal for his outstanding contributions to the development of international scientific cooperation in the field of space research. Professor Steve Buckman was awarded a Fulbright Senior Fellowship enabling him to pursue research at the University of California, San Diego, while taking full advantage of the A$-US$ exchange rate. Dr Brenton Lewis was elected as a Fellow of the Institute of Physics (UK), and was awarded the DSc degree of the University of Adelaide for his research achievements at the ANU. Dr Anatoli Kheifets was honoured by the holding of the Anatoli Kheifets Workshop on Multi-Electron Processes in Atoms at the Photon Factory, Japan.

A summary of the various research activities in the Department follows:

Low-Energy Electron Scattering and Spectroscopy

This year, the magnesium atom has been the main target in the study of temporary negative-ion formation and decay in electron-Group II atom collisions. The emphasis has been on the autoionising energy region above the ionisation limit (9.36 eV), where multiply excited resonances may be expected to occur. The presence of resonances in elastic scattering has been observed through the detection of electrons detached into the elastic scattering channel during the decay of a resonance. Detachment into an excited-state channel has been observed by detecting radiation from the de-excitation of the $^3P_1$ state to the ground $^3S_0$ state. A final series of measurements on mercury has also been undertaken in order to provide some further information on lower-lying resonance states. *(R. Panajotovic and S.J. Buckman)*

Extensive measurements of absolute cross section for the scattering of electrons from sulphur hexafluoride (SF_6) have been performed over a large energy range (2.7 to 75 eV). The main aims of these measurements were to confirm (or otherwise) a hypothesis that several of the earlier measurements available in the literature underestimate the integral elastic cross section. This experimental study utilised a novel magnetic scattering angle-changing device to obtain, for the first time, absolute differential cross sections for backward scattering angles (135° to 180°), previously unattainable due to mechanical constraints of the spectrometer. Modifications to the apparatus were made at the conclusion of the above measurements to incorporate differential pumping around the electron spectrometer, which will reduce exposure of the spectrometer to the target gas of interest. This modification will enable the measurement of cross sections from reactive molecular species, such as those used in plasma processing devices. *(H. Cho [Chungnam National University, Korea], R.J. Gulley and S.J. Buckman)*

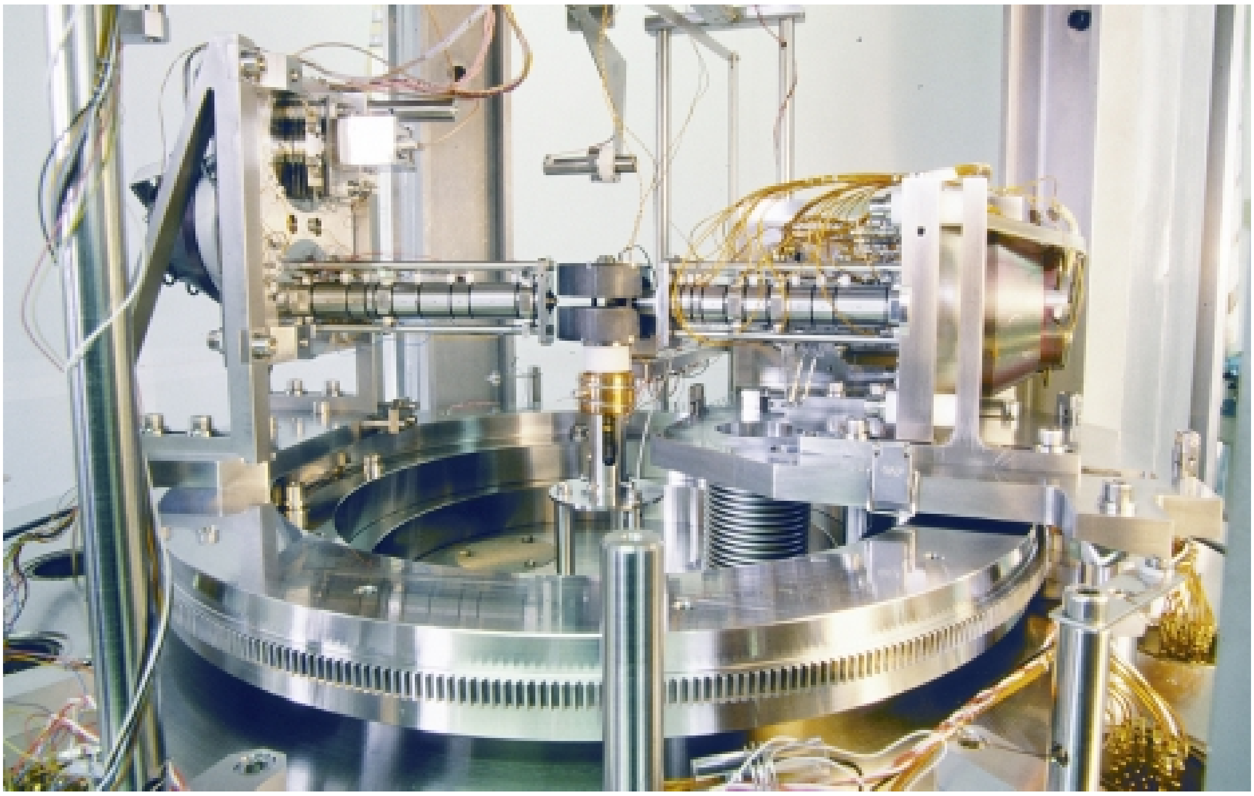
Studies of absolute inelastic cross sections at near-threshold electron energies using conventional techniques have resulted in measurements with large variations and uncertainties, mainly due to the difficulties involved in characterising the transmission function of the scattered-electron energy analyser. A time-of-flight analyser, which is presently in the testing phase, has a transmission function that is essentially independent of the energy of the scattered electron, and has the potential to enable the measurement of inelastic differential cross sections at near-threshold energies which were previously unattainable. This device can also be used to calibrate the transmission function of the existing electron-energy analysers. *(A.J. Daley, L.J. Uhlmann, R.J. Gulley and S.J. Buckman)*

Assembly of the recoil-atom spectrometer, which is designed for the measurement of absolute cross sections for electron scattering from metastable helium, has been completed and it will soon be attached to the metastable-atom beam line (see Atom Manipulation Project). *(L.J. Uhlmann, R.J. Gulley and S.J. Buckman)*

A set of electron scattering cross sections for molecules has been completed for a new edition of the Landolt-Bornstein Tables. *(M.T. Elford, S.J. Buckman and M.J. Brunger [Flinders University])*

Electron Momentum Spectroscopy of Solids (EMS)

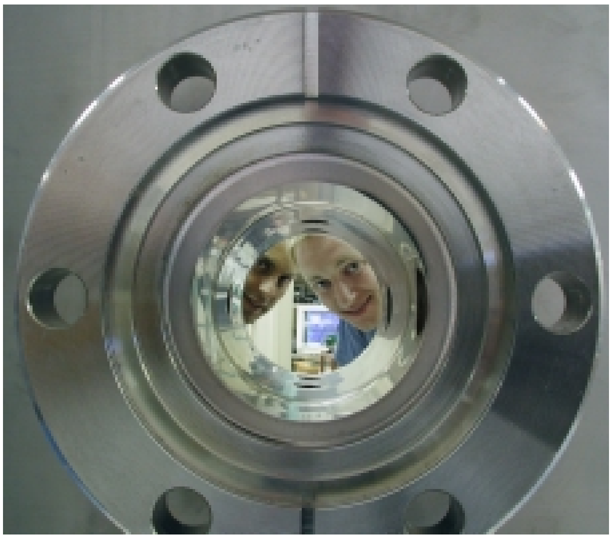
The high-energy spectrometer is providing us with measurements of the spectral function of materials with high clarity. The momentum resolution of the spectrometer exceeds the design specifications. The results of the spectrometer were cross-calibrated with those obtained by (γ,eγ) spectroscopy in collaboration with the group of Professor Friedhelm Bell using graphite targets. Methods for the fabrication of thin targets were



The Crossed Beam Apparatus (CBA)

tested, and thin aluminum, copper and gold foils were prepared and measured successfully. The quality of these data brings electron momentum spectroscopy of solids to a new level. The fact that, even for gold, we obtain very clear spectral momentum densities means that at high energies the EMS technique is not restricted to light elements only.

Full many-body calculations were performed for graphite and aluminium. These calculations describe the data much better than the traditional band-structure type calculations. Extension of these calculations to transition metals is planned. Preparation of single crystal thin films and improvement of the energy resolution are planned on the experimental side. *(M. Vos, A.S. Kheifets and E. Weigold)*

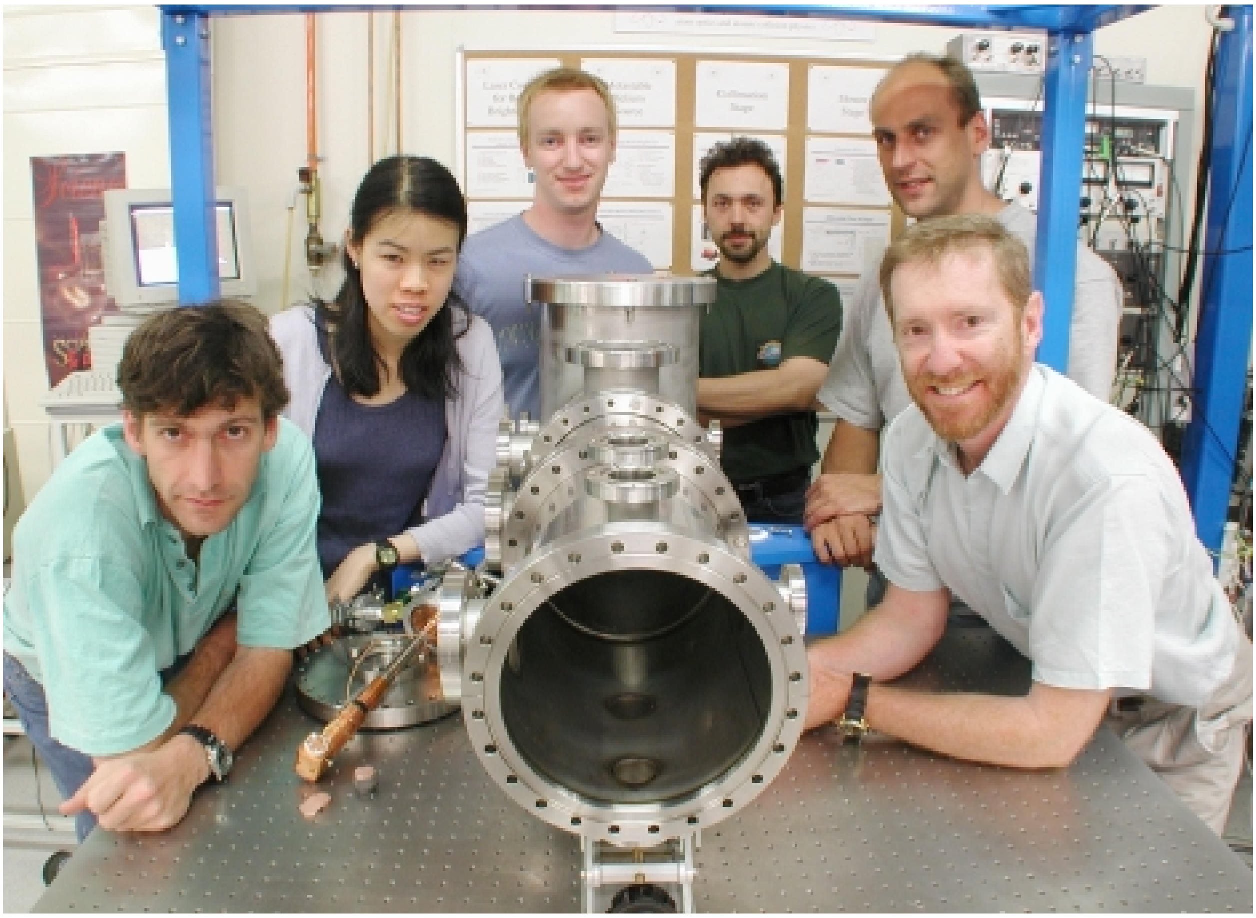


Looking down the beam line

Atoms, Molecules, Radiation, and the Nanoworld

In investigations of the interaction of radiation with matter, studies of mechanisms for latent track registration (the physics of particle detectors), and the atomic and molecular physics of condensed matter phase changes, have been continued. Experiments (TEM) on the production of radiation damage in single crystals of silicon, graphite, fluorite and yttrium iron garnet by fission fragments, GeV heavy ions, and MeV cluster ions have been compared and contrasted. Theories (thermal spikes) of track formation based on direct "melting" into an amorphous state (or other irreversible phase transitions), on linear and macroscopic thermodynamics of immediate electron/lattice energy transfer, and on time-attenuated Gaussian temperature distributions fail to describe radiation damage processes in different targets.

We have shown (with Dr Dietmar Fink, HMI, Berlin) that specific crystal lattice properties determine the nature of the latent track. For silicon and graphite a mechanism of particle activated prompt anneal takes place. A reverse cooling and annealing wave allows recovery by epitaxy of the primary "random" disorder. Radiation enhanced recovery processes also play a role (the divacancy in silicon). For fluorite and lithium fluoride targets (with Dr Christina Trautmann, GSI, Darmstadt) the one-dimensional <100> dynamics (and later, diffusion) of molecular crowdions on the anion sublattice (Vh centres) creates a linear intermittent



The new helium cooled, metastable helium beam line and members of the Atom Manipulation Project array of faceted metallic colloids on the projectile trajectory. Only in the complex case of yttrium iron garnet does the track "width" have meaning.

Bragg's rule (1905) for the additivity of electronic stopping due to the atomic components of a compound target, considered "random", fails for real crystals. The orientation of the target, and of the projectile – for molecular and cluster (e.g., C_{60}) projectiles (with Professor Eugene Gamaly, Applied Mathematics) – also strongly influences latent track features.

Comprehensive experimental results on the angular dependence of the differential cross section for elastic scattering of low energy electrons (0-10 eV) from diatomic molecules (e.g., N_2), and of the energy dependence of the total cross section reveal, for the first time, the presence of a double "rainbow" – a consequence of sequential scattering (with Professor Steve Buckman). For diatomic molecules the electron wave is attractively screened-Coulomb scattered from the first atom, and focused onto the second (with Professor Salvador Cruz, Ixtapalapa, Mexico)

Studies of nanomolecular self assembly of new nanostructures, including dodecahedral C_{20} (pentagons only) and nanotubes, have been extended. Calculations of the characteristic axisymmetric vibrations of C_{20} (infra-red and Raman modes), based on simple continuum shell and finite element models are in progress (with Dr Alexander Berdinsky, Novosibirsk).

In formation of carbon and boron nitride nanotubes (with Professor Jim Williams and Dr Chen Ying, EME) in ball-milling (nucleation) and annealing (growth), the roles played by homogeneous and heterogeneous nucleation have been studied using chemical reaction rate theory. It has been shown, from the thermodynamics of the capillarity of solids, that "bamboo" nanotubes owe their internal structures both to heterogeneous growth of the tube and of the foreign (metal) endohedral precipitate itself. *(L.T. Chadderton)*

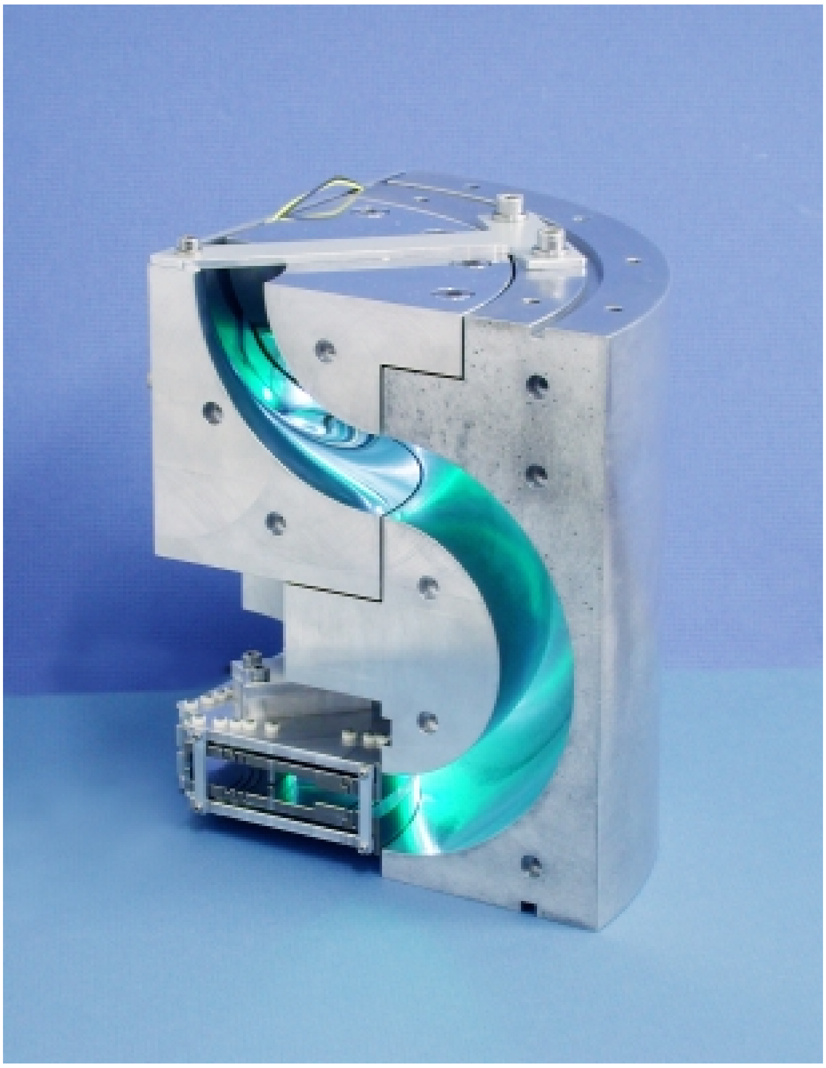
Atom Manipulation

The atom trap facility developed in the Atom Manipulation Project has been used to study electron collisions with metastable helium atoms. Approximately 20 million helium atoms in the 2^3S_1 state are confined by laser light forces in a magneto-optic trap 5 mm in diameter at temperatures less than 1 mK. We have employed RF spectroscopy at the 1083 nm 2^3S_1 - 2^3P_2 trapping transition to measure the line-integrated trap density and determine the trap loss rate due to electron collisions from a monoenergetic electron gun in the range 10 - 50 eV. This will enable total electron scattering cross sections for this important metastable species to be determined for the first time.

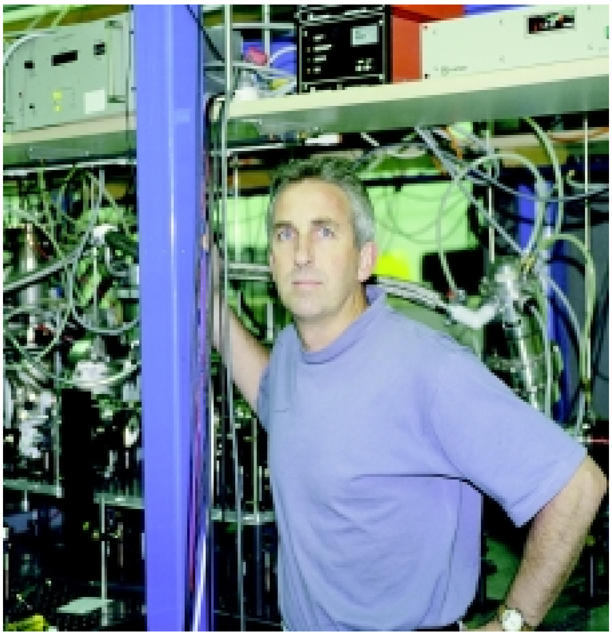
Presently, the atom trap is loaded from a bright metastable helium beam line, which is operated using a helium discharge source at liquid nitrogen temperatures. Funding this year from an ANU Major Equipment Grant has allowed the construction of a second source of metastable helium atoms operating at liquid helium temperatures, which reduces the need for laser slowing of the generated atoms. This second source uses a continuous flow, liquid helium cryostat to cool the discharge source to <10 K. It is now undergoing initial characterisation tests using a third metastable helium beam apparatus that has been developed as a testing rig and for experiments on atom lithography. When completed, the cryogenic source will be used exclusively for loading the atom trap, which will free up the beam line for other atom optics and atomic collision physics experiments. *(M.D. Hoogerland, M. Colla, R.G. Dall, R.J. Gulley, R. Heck, J. Swansson, L.J. Uhlmann, S.J. Buckman and K.G.H. Baldwin [LPC])*

Spin Resolved (e-2e) Studies on Laser Excited Atoms

To understand the origins of the diversity of forms and properties of matter requires understanding, on a microscopic scale, the behaviour of atoms which are the basic building blocks of matter. This demands a detailed knowledge of both their internal electronic structure and the way in which they interact with their



A section of the advanced electron energy analyser built in the School workshops. The analyser is used to investigate atomic collision processes



Professor Stephen Buckman was one of only two recipients of a Fulbright Senior Scholarship in this year's round

surroundings, be that with other atoms, charged particles or electromagnetic radiation. Our experiments involve crossing beams of isolated atoms with beams of electrons, and energy- and momentum-analysing the resulting scattered electrons in sophisticated analysers. In contrast to conventional scattering experiments, our measurements are highly quantum-state specific, using lasers to prepare the spin and orbital angular momentum states of the reaction participants. The results of such measurements yield detailed information on atomic structure, reaction rates and underlying mechanisms driving atomic collision processes. This information is vital to the development and optimisation of numerous devices of technological importance such as lasers, gas discharges and plasmas which rely upon accurate data from these experiments.

In our earlier experiments with spin-polarised electrons and spin-polarised target atoms we demonstrated the power of our experimental techniques by confirming the existence of previously postulated mechanisms underlying the process of electron impact ionisation. Nevertheless, although using the best available technology, the count rates encountered in those measurements were low, limiting the stringency of tests which they could provide to theory. To address this limitation we have designed and constructed a new generation of toroidal electrostatic analysers which will dramatically increase the speed of future measurements. To incorporate these new analysers, we have had to completely redesign and rebuild our experimental apparatus this year. As a result of the modifications we have made, including the incorporation of state-of-the-art high speed delay-line detectors and improved target collimation, improvements in the speed of experiments of up to three orders of magnitude are anticipated, at no cost to energy or momentum resolution. Using the unparalleled sensitivity of the modified apparatus, experiments involving the search for relativistic effects in the ionisation of heavy atoms and the investigation of inner shell ionisation processes are soon to be performed which lie beyond the sensitivity of existing devices. *(J.C.A. Lower and E. Weigold)*

Theory of Atomic Double Ionisation

Atomic double photoionisation is one of the most fundamental and intriguing problems of atomic collision physics. Driven entirely by many-electron correlations, this process requires the highest degree of sophistication from theoretical models. Application of the convergent close-coupling (CCC) theory to atomic double ionisation has been a spectacular success. Angular correlation and energy sharing between the two photoelectrons as well as the circular dichroism in helium double photoionisation were predicted by the CCC model with high accuracy, and subsequently confirmed in a large number of recent experiments at various synchrotron radiation sources in Japan, UK and USA.

Further development of the theory, based on the *B*-spline technique, is currently underway. It will allow the description of double photoionisation from closed-shell atomic targets such as noble gas atoms. *(A.S. Kheifets, I. Bray [Flinders University] and A. Ipatov [St. Petersburg Technical University])*

Theory of Many-Electron Correlations in Solids

Ab initio calculations of excited states of solids have gained a lot of interest due to the feasibility of performing such calculations, since the advent of high-performance computers. Experimentally, a wealth of information about such states can be obtained by means of ionisation spectroscopy after removing an electron from the correlated electron ensemble in a solid.

A suitable method for studying excited-state properties of extended systems is the Green's function method. To calculate the Green's function, one requires the self-energy operator which is non-local and energy dependent. The simplest approximation for the self-energy beyond the Hartree-Fock approximation that takes into account screening is the GW approximation. This approximation can incorporate a realistic crystalline structure. Further vertex correlations to the GW approximation in the form of the cumulant expansion are now also possible. On this basis, the satellite structure in the ionisation spectra of solids was simulated and found to be in excellent agreement with the recent experimental data from the electron momentum spectroscopy group at AMPL. *(A.S. Kheifets and F. Aryasetiawan [University of Lund])*

Inverse Scattering Theory

Development was completed of a new technique for phase-shift analysis in multi-channel scattering in which the complete scattering matrix could be extracted from the experimentally measured differential cross section. This technique made use of the unitarity condition on the scattering matrix and was applied to the interaction of two spinless particles. *(A. Purwanto, D.R. Lun, R.P. McEachran and S.J. Buckman)*

Atomic Scattering Theory

The relativistic distorted-wave method has been used to study the electron-impact excitation of both Th and Pb. Results for spin polarisation parameters, as well as the differential cross sections, were determined. The overall agreement with available experimental measurements was quite satisfactory.

Similar calculations for the D states of Mg and for the Group IV elements have now been completed and a new program for studying the excitation of heavy ions has been commenced. *(R.P.*

McEachran, A.D. Stauffer [York University] and R. Srivastava [Roorkee University])*

Positron Interactions with Atoms

The elastic cross section for positron scattering from Xe has been determined by the polarised-orbital method while the corresponding excitation and ionisation cross sections have been determined within a distorted-wave framework in an energy range up to 200 eV. The relative contributions of these individual cross sections to the total cross section were analysed and compared with recent experimental measurements. The overall agreement with experiment is quite satisfactory except in the threshold region. *(R.P. McEachran, L.A. Parcell [Macquarie University], R.I. Campeanu [Seneca College, Toronto] and A.D. Stauffer [York University])*

The elastic and ionisation cross sections for positron scattering from Kr and Xe were determined in an energy range up to 400 eV. A new model for treating ionisation was developed and the overall agreement with experiment is again quite satisfactory. *(R.P. McEachran, R.I. Campeanu [Seneca College, Toronto] and A.D. Stauffer [York University])*

Diffusion of Meteor Trails

The study of the diffusion of electrons in meteor trails that commenced in 1997 has continued during 2000. The study represents a collaboration between the ANU, the University of Adelaide and James Cook University. *(M.T. Elford, K. Kumar [TP], W.G. Elford [University of Adelaide] and R. Robson [James Cook University])*

VUV Spectroscopy

Work has continued on the measurement of photodissociation cross sections of relevance to various atmospheric, aeronomic, and astrophysical processes, using both conventional and high-resolution laser-spectroscopic techniques.

Using the 2.2 m monochromator system, evidence has been uncovered of the existence of the magnetic-dipole transition $^3\Pi_g$ -$X^3\Sigma_g$-underlying the electric-dipole-allowed Schumann-Runge system of O_2. It had been predicted theoretically that this transition would be too weak to be seen, or to play a role in this atmospherically-important region of the O_2 spectrum. *(B.R. Lewis, S.T. Gibson and E.H. Roberts)*

The continuing program of high resolution (Doppler limited) VUV laser spectroscopy on the oxygen Schumann-Runge band system is probing increasingly higher vibrational levels near the dissociation limit at 175 nm. The complexity of the spectral lines near the continuum is enriched by perturbations between coincident energy levels in different states which have already led to the identification of two new states of diatomic oxygen. When complete, this study will yield a definitive assignment of the spectrum of this important atmospheric band system. *(K. Waring, B.R. Lewis, S.T Gibson and K. Baldwin [LPC])*

Work continues on the development of an injection-seeded solid-state laser system intended to yield a bandwidth significantly less than 0.1 cm^{-1} full-width at half-maximum (currently achieved by our excimer-pumped systems) that can be employed in our VUV laser-spectroscopic studies. This is a joint program with Professor Brian Orr, of Macquarie University, relying on RIEF and ARC funding. *(K.G.H. Baldwin [LPC], B.J. Orr [Macquarie University] and B.R. Lewis)*

Electron Energy-Loss Spectra (EELS)

The large changes in the relative intensities of vibrational features in the optically-allowed transitions in the EELS of O_2, as the scattering conditions were varied, were analysed and explained by employing the concept of the "generalised electronic transition moment" in coupled-channels calculations of the EELS for the interacting Rydberg and valence states of O_2. Similar work is continuing on the optically-forbidden transitions. *(B.R. Lewis, S.T. Gibson, M.J. Brunger [Flinders University] and M. Allan [University of Fribourg])*

Resonance-Enhanced Multiphoton Ionisation (REMPI)

New, properly calibrated (2+1)-photon REMPI spectra from the metastable $a^1\Delta_g$ and $b^1\Sigma_g^+$ states of O_2 have been acquired and analysed rotationally, yielding the first accurate experimental

Steve Buckman's Fulbright award leads to a flurry of applications for the post of Acting Head during his absence information on strong perturbations in the Rydberg $d^1\Pi_g$ state. This information will be used to optimise a new coupled-channel treatment of the $^1\Pi_g$ Rydberg-valence interactions in O_2. *(B.R. Lewis, S.T. Gibson, R.A. Copeland [SRI International, California], M.L. Ginter [University of Maryland] and J.S. Morrill [Naval Research Laboratory, Washington DC])*

Analysis is continuing on interesting interference effects observed in (3+1)-photon REMPI spectra from the $X^3\Sigma_g^-$ state of O_2 which vary with the gas pressure. These are nonlinear effects arising due to interference between the (1+1) and (3+1) transition amplitudes. *(B.R. Lewis, S.T. Gibson, K.G.H. Baldwin [LPC] and R.A. Copeland [SRI International, California])*

A unique example of completely destructive quantum interference between two resonances interacting through an optically-inactive continuum has been discovered in the (2+1)-photon REMPI spectrum from the $b^1\Sigma_g^+$ state of O_2, acquired in an optical-optical double-resonance experiment. The interference effect was verified through coupled-channel calculations which showed that the complex predissociative interactions reduced effectively to a simple two-resonance interaction treatable by the classical Fano-Mies configuration-interaction (CI) theory. *(B.R. Lewis, S.T. Gibson; R.J. Donovan and K.P. Lawley [University of Edinburgh])*

Atmospheric Computation

Work has continued on an ARC-funded project involving quantum-mechanical modelling of the transmission of solar VUV radiation through the terrestrial atmosphere. A sum rule involving the lineshape asymmetry which was discovered during the course of this project has been extended to the case of weak molecular predissociation by optically-active continua and a treatment based on CI theory has been shown to give results identical to those implied by a full coupled-channel treatment. Considerable progress has been made towards the ultimate aim of the project, i.e. to produce a comprehensive database to be used extensively by the community of atmospheric geophysicists in their photochemical models. Preliminary results of the computational model were presented in an invited talk at the XXV Symposium of the European Geophysical Society. The atmospheric transmission calculations will be tested against new, high-resolution cross sections obtained in our VUV laser-spectroscopy laboratories. These measurements will be the first to be performed under the new strategic initiative STEP, facilitated by the appointment of a new Postdoctoral Fellow in 2001. *(B.R. Lewis, S.T. Gibson; L.W. Torop and F.T. Hawes [Adelaide University])*

Photodissociation Dynamics

The construction of the Coincidence Photofragment/Photodetachment Spectrometer is nearing completion. This instrument combines a number of technologies, including plasma, ion, electron and laser physics for the purpose of studying the photodissociation dynamics of molecular radicals.

The anion beam line of this instrument has been established and the crucial ability to isolate specific mass ion radicals has been verified. A novel gating, bunching and potential referencing unit has been designed, constructed and verified to yield a mass resolving power of more than 300.

The first experimental photodetachment stage will be completed with the installation of a time-of-flight photoelectron detector. *(S.T. Gibson, E.H. Roberts, B.R. Lewis and S.J. Buckman)*

Atmospheric Evolution and Climate Change

A CO_2 weathering model has been used to explore major steps in the evolution of the Earth's climate as the Sun steadily brightened throughout geologic time. The model balances the contributions to the surface temperature from an increasing solar

Staff and students of the Atomic and Molecular Physics Laboratory flux, a generally diminishing CO_2-H_2O palaeo-greenhouse and a planetary surface subject to changes in weathering and other physical and biological evolutionary processes.

The model calculations use 1-D radiative convective techniques and seek to identify major climate changes only. The results can be described in terms of three qualitatively different Mega-Climates. Mega-Climate 1, with its high, but rapidly declining, Archean surface temperature resulted from high atmospheric CO_2 content, rapid early outgassing and low weathering rates on a largely water-covered planet. Mega-Climate 2 began about 3 Gyr ago when temperatures began to fall as major continental land masses developed, increasing weathering rates, depleting atmospheric CO_2, and producing the first Precambrian glaciations about 2.3 Gyr ago. During Mega-Climate 2 evolutionary biological processes increased the surface weatherability in incremental steps starting about 1 Gyr ago with the proliferation of life forms that marked the transition from the Proterozoic to the Phanerozoic, and the CO_2 gas emission rate was modulated by plate tectonics driven by convective cycling in the mantle (the Phanerozoic Supercycle). The PSC has a period of about 300 Myr with gas emission maxima at both the open (rifting) and closed (Pangea) limits of the PSC and gas emission minima on both the closing and opening sides of the cycle with a gas period of about 150 Myr. Modulation of the gas emission rate in this way accounts for the remarkable regularity in the occurrence of major glaciations between 300 and 900 Myr BP. Including additional weathering in the model due to the formation of the Tibetan plateau can explain the late Cenozoic glaciation at about 25 Myr BP.

Extending the model to the future suggests that the CO_2 control system would not be sufficient if the Sun continues to brighten. The present level of CO_2 is already so small that further reduction in CO_2 cannot protect the Earth from Mega-Climate 3 with steadily increasing surface temperatures caused by the continued brightening of the Sun. In the long term (the next Gyr) the main danger to the biosphere may come from a decreasing rather than an increasing atmospheric CO_2 level.

We note that, according to the model, the "natural" changes that occurred in the atmospheric CO_2 level over geologic time were much larger than the doubling that may result from continued "industrial" development at present levels. *(J.H. Carver and I.M. Vardavas [University of Crete])*

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Professor and Head of Laboratories

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Professor

Erich Weigold, BSc Adel, PhD, FAA, FTSE, FAPS, FAIP

Adjunct Professors

Lew Chadderton, DSc Dur, MA PhD Camb, C Phys, FInstP, FAIP

Bob McEachran, MSc PhD UWO, C Phys, FinstP

Senior Fellow and Acting Head of Laboratories (from September)

Brenton Lewis, PhD DSc Adel, C Phys, FInstP, FAIP (Head, Ultraviolet Physics Unit)

Fellows

Hyuck Cho, BSc Sog, PhD Ariz (until June) (ARC IREX Fellowship)

Stephen Gibson, BSc PhD Adel

Anatoli Kheifets, BSc PhD St. Pet (jointly with Theoretical Physics)

Maarten Vos, MSc PhD Gron

Maarten Hoogerland, MSc Leid, PhD Eind

Research Fellow

Julian Lower, BSc PhD Flind

Postdoctoral Fellows

Alan Lun, BSc Zhong, PhD Melb (until September) (ARC Fellowship)

Robert Gulley, BSc Qld, PhD (ARC Fellowship)

Radmila Panajotovic, MSc PhD Belgr

Adjunct Fellow

Fred Hawes, BA ME Rice, PhD Flor (ARC Research Associate, U. Adelaide)

Visiting Fellows

Chris Brion, BSc PhD Brist, FRSC, FCIC (November-December)

John Carver, MSc Syd, PhD ScD Camb, AM, FAA, FTS, FAIP (Emeritus Professor)

Robert Crompton, BSc PhD Adel, AM, FAA, FAIP, FInstP, FAPS (Emeritus Professor)

Salvador Cruz, MSc PhD UNAM (July-August)

Malcolm Elford, BSc PhD Adel

Andrei Ipatov, PhD St Pet Tech (jointly with Theoretical Physics, until May)

Mitsu Kono, MS Kyoto IT, PhD Grad U Adv Sci (from April)

Fred Mies, BS CCNY, PhD Brown, FAPS (February)

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Kevin Roberts, MechTechCert SAIT

Departmental Administrator

Alice Duncanson

Electronic Materials Engineering

Professor Chennupati Jagadish - Head of Electronic Materials Engineering

http://wwwrsphysse.anu.edu.au/eme

The Department of Electronic Materials Engineering conducts interdisciplinary research on the physics and engineering of electronic and optoelectronic materials and devices.

Research Summary

EME's research performance in 2000 is measured by more than 80 high quality refereed journal or conference papers, 12 invited keynote conference presentations, success with competitive ARC programs and with other grants and fellowships. Other measures of recognition for EME personnel were seven staff promotions, several staff and student awards and Chairmanship of major international conferences. There were also major steps taken to commercialise EME's laser devices through the establishment of a spin-off company. Research highlights extended across all the department's pursuits. In silicon, the work on cavities and voids has uncovered new physical processes that have led to a much improved understanding of the formation and properties of open volume defects. The nanocrystal research has also made great strides in 2000, providing insights into the role of hydrogen and other impurities in enhancing luminescence. The understanding of how oxides and nitrides form during low energy ion bombardment in secondary ion mass spectrometry (SIMS) analysis has also been dramatically advanced. There were two projects involving the use of synchrotron radiation in 2000, one addressing surface desorption of various elemental species under photon irradiation and the other involving extended X-ray absorption fine structure analysis of disordered semiconductors. The former study has shown a preferential bonding of hydrogen to As in GaAs, whereas the latter has led to the most detailed description to date of the non-stoichiometry and local atomic structure in amorphous semiconductors. A range of new behaviour was discovered in ion bombarded gallium nitride, including the observation of planar defects, highly porous amorphous gallium nitride and dramatic surface erosion during elevated temperature bombardment. Research on carbon nanotubes explored a new, entirely solid state process for tubular formation and made significant progress in understanding the mechanisms for nanotube nucleation and growth. In the areas of growth and processing of III-V compound semiconductors, successful quantum well infra-red photodetector structures were fabricated and a process was developed (and patented) for tuning their wavelength. In the devices area, vertical cavity surface emitting lasers were fabricated at 850 nm and a process developed and patented for producing steerable devices. Single mode 980 nm pump lasers were grown, processed and mounted and these devices exhibit state-of-the-art performance. In ion beam analysis, the highly sensitive elastic recoil detection analysis method, developed jointly with the Department of Nuclear Physics, continued to be improved and exploited for a range of thin film applications. Finally, studies of nanoindentation behaviour in a range of semiconductors have identified, for the first time, the complete sequence of deformation processes in these materials.

EME's already extensive research facilities were considerably enhanced in 2000 with the installation of two major equipment items funded by the ARC RIEF program. A new Aixtron metalorganic chemical vapour deposition (MOCVD) system was installed and commissioned to grow a range of gallium arsenide and indium phosphide based heterostructures. This machine was calibrated in record time and has already grown top quality structures for infrared photodetectors and lasers. The second facility is a new tandem accelerator for ion beam analysis, which has replaced the old Van de Graaff (1962-2000). This machine operates with a terminal voltage of 1.7 MV, thus allowing a much wider range of analytical capabilities than was previously possible. For example, since calibration it has been undertaking Rutherford backscattering analysis of a wide range of samples using a He^{++} beam with energies up to 5.1 MeV. Both facilities required extensive laboratory reconstruction and in-house assembly, largely carried out by EME's highly skilled technical staff. Indeed, EME's excellent facilities, which are superbly maintained to give a minimum of down time, are a credit to such technical staff (Michael Aggett, Tom Halstead, Alan Hayes, Bernie King, David Llewellyn and

Antony Watt) and technical assistants (Martin Conway and Antony Williams). EME would also like to acknowledge the crucial role played by the School's workshops and service areas in the installation of its new facilities, particularly Dennis Gibson for the design and installation of the computer control system for the MOCVD laboratory.

There were again a number of staff and student highlights during the year. Professor Chennupati Jagadish won the prestigious millennium medal of the IEEE and also was elected to the Nanotechnology Technical Committee of the IEEE Electron Devices Society. Dr Rob Elliman was elected as Vice-President of the Australian Institute of Physics and Dr Mark Ridgway was appointed as a member of the Specialist Committee of the Australian Synchrotron Research Program. Dr Hoe Tan and Sanju Deenapanray were successful in obtaining a QEII fellowship and a post-doctoral fellowship from ARC, respectively. Fu Lan won the LEOS graduate student fellowship and also presented EME's student talk for the John Carver prize. Annette Dowd and Jodie Bradby won best poster prizes at the Australian Electron Microscopy Conference. Rob van der Heijden won a best poster prize at COMMAD 2000, held in Melbourne 5-8 December. EME was also extremely successful with promotions and reclassifications of staff in 2000. Michael Aggett, Alan Hayes, Bernie King, and Drs Ying Chen, Mladen Petravic, Mark Ridgway and Heiko Timmers deserve hearty congratulations.

Under the Chairmanship of Professor Chennupati Jagadish, EME hosted the 11th International Semiconducting and Insulating Materials Conference in Canberra in July. There were around 80 participants at this meeting, mostly from overseas, and the success of this event further raised the profile of EME's research effort. In addition, Dr Rob Elliman will chair another international meeting, the 15th Ion Beam Analysis conference, which will be held in Cairns in July 2001. These invitations, as well as the steady stream of international visitors (17 in 2000) to EME, is evidence of the high international regard for EME's research.

Finally, the Department could not have functioned without its departmental administrator (Laura Walmsley), who not only took care of EME's staff and students, endless visitors, reports, budgets, organised conferences and managed the administration of external grants, but was also the main social organiser. In addition, the School's administrative and public relations staff members are also acknowledged for their important contribution to the smooth running of the Department.

The research highlights below are arranged into the four basic pursuits in the department.

Ion Beam Synthesis/Modification of Materials

Nanocrystalline Si exhibits strong room-temperature luminescence. However, as formed, many nanocrystals contain non-radiative defects which reduce the luminescence efficiency. Hydrogen passivation of the defects improves the luminescence efficiency and has been the subject of study over the past year. It has been shown that passivation preferentially increases the luminescence from larger nanocrystals. This process is reversible, with emission spectra returning to their pre-passivation form when H is removed from the samples by annealing. This confirmed that passivation did not affect the physical particle size distribution but only distribution of optically active nanocrystals. This has important implications for the comparison of experimental data with the predictions of quantum confinement theories. In addition, the effect of P, Ge and N on the luminescence intensity, spectral distribution and physical size distribution of silicon nanocrystals was examined. All impurities were found to affect the luminescence intensity, with P and Ge tending to decrease the intensity when present at 10-30% of the excess Si content. Significantly, N was found to increase the emission intensity in the range 5-30%. The low solubility of N in silicon suggests that the N remains in the surrounding silica. *(S. Cheylan, N. Smith, D. Llewellyn and R.G. Elliman)*

Semiconductor-doped glasses exhibit interesting optical properties and have long been of both scientific and technological interest. For example, the optical absorption of such glasses depends strongly on the composition of the semiconductor dopant, a feature that has led to their use as high quality optical filters. Our work in this area has been involved with the nonlinear optical response of Ge implanted silica. Extensive physical characterisation of the material has shown that the magnitude and temporal response of the optical nonlinearity is insensitive to the form of the implanted Ge. Indeed, similar responses are observed for samples containing amorphous or crystalline Ge. The response does however depend on the presence of Ge and is much larger for Ge implanted silica than for Si implanted silica. This has led to the conclusion that the nonlinear response is associated with a Ge-related defect centre. *(A.R. Dowd, D. Llewellyn, M. Samoc [LPC], B. Luther-Davies [LPC] and R.G. Elliman)*

Ion irradiation of germanium at room temperature is known to produce a porous or sponge-like surface layer, an effect that is not usually observed in silicon. The mechanism responsible for this morphological transformation is unclear and the interpretation of previous experiments is difficult because they often involve the implantation of foreign species or irradiation of the near-surface only. To overcome these limitations, experiments were undertaken using high-energy self-ion irradiation. The substrate temperature was also varied to assess its impact on the transformation. Pronounced swelling of the irradiated material was evident for temperatures between -50°C and 200°C, the process was insensitive to temperature in this range and exhibited an approximately linear dose-dependence for doses up to $1x10^{17}$ $Ge.cm^{-2}$. For temperatures outside this range, only sputtering effects were observed. The structure of the porous surface layer was examined by transmission electron microscopy (TEM) and for samples irradiated at 22^{o}C, it was shown to have a density ~30% that of bulk Ge. These layers were further shown to be stable during subsequent annealing to 500^{o}C. *(B. Stritzker, J. Zou [University of Sydney] and R.G. Elliman)*

Extended X-ray absorption fine structure measurements continue to yield insight, at the atomic-scale, of the implantation-induced structural evolution of the amorphous phase in materials such as Ge, InP and GaAs. Experiments were performed at both the Photon Factory, Japan and the Stanford Synchrotron Radiation Laboratory, USA. In the absence of porosity, the inter-atomic distance distribution of *amorphous* Ge was shown to evolve as functions of both the ion dose and implant temperature. The changes in structural parameters were attributed to increased fractions of non-four-fold coordinated atoms as a means of accommodating implantation-induced defects in the amorphous phase. Following thermally-induced structural relaxation, the observed reduction in non-Gaussian static disorder was consistent with a reduction in the non-four-fold coordinated atom fraction of the amorphous phase. Raman measurements confirm this interpretation. *(M.C. Ridgway, C.J. Glover, G. Azevedo, G.J. Foran [ANSTO], K.M. Yu [Lawrence Berkeley National Laboratory] and D. Desnica-Frankovic [Boskovic Institute, Croatia])*

In collaboration with the Department of Nuclear Physics and the University of Bonn, perturbed angular correlation was utilised to characterise In-probe/point-defect complexes in ion-implanted Ge. The ion dose and Fermi level dependence of two distinct probe environments were measured as a means of identifying the defective configurations. *(C.J. Glover, M.C. Ridgway, A.P. Byrne [NP] and R. Vianden [University of Bonn])*

Further experimental and theoretical progress has been achieved toward an understanding of the implantation-induced cracking of silica. A multitude of potential influences have been considered and measurements of the implant condition dependencies have been utilised to determine the relative significance of individual mechanisms. *(C.M. Johnson, M.C. Ridgway and V. Gurarie [Melbourne University])*

TEM was used to examine defect formation in Si implanted with MeV Sn ions at different implant temperatures in the sub-amorphous dose regime. The study revealed a drastic change in microstructure with implant temperature. Two types of dislocation loops were observed in some samples, namely the perfect loop and the faulted loop. Dislocation loop formation was suppressed in samples implanted at elevated temperature where only {311} rod-like defects were observed. All the defects observed were identified to be interstitial in nature. Further, a higher proportion of perfect loops was observed with lower implant temperatures. These results indicate a hierarchy of defect formation in implantation induced defects which is believed to be a result of the extent of dynamic annealing. *(J. Wong-Leung, C. Jagadish and J. Fitz Gerald [RSES])*

The behaviour of deep, narrow amorphous volumes constrained by a crystalline substrate have been examined using TEM. These amorphous wells have been created by ion-implantation through a mask using the NEC tandem ion-implanter at EME. The amorphous volume is transformed at the vertical and lateral interfaces into single crystal with the same orientation as the substrate when it is annealed. The fast growth directions coincide with the [100] directions in the crystal. The recovered crystal is not pristine, with many secondary structures resulting from the process. *(A.C.Y. Liu and J.C. McCallum [Melbourne University] and J. Wong-Leung)*

In a collaborative project with the CNRS, Orsay, France, the interaction of irradiation-induced defects with nanocavities was studied using both in-situ and ex-situ TEM and Rutherford Backscattering Chanelling (RBS/C). Depending on irradiation temperature, cavities were either observed to be preferential nucleation sites for amorphisation or sinks for diffusing silicon interstitials. In the former process it was proposed that, since amorphisation results in an expansion of the surrounding lattice and hence a free energy increase, cavities are favoured sites for nucleation of the amorphous phase. Indeed, the amorphous phase is plastic and can expand into the cavity volume without straining the surrounding lattice. At higher irradiation temperatures, interstitials are mobile and can annihilate at cavities, leaving a zone around cavities that is defect-free. At temperatures where amorphous layers are formed, cavities are found to shrink and disappear. This effect has only a small temperature dependence but the diameter of the cavities is found to decrease linearly with ion dose. This behaviour suggests that ion-induced plastic flow is responsible for the shrinkage process. Two invited papers were delivered at international meetings on this topic during 2000. *(J.S. Williams, X.F. Zhu, M.C. Ridgway, M.J. Conway;F. Fortuna, H. Bernas and M-O. Rouault [CNRS])*

Ion beam induced epitaxial crystallisation of amorphous silicon was studied in some detail in an attempt to shed more light on the mechanism of crystallisation. In-situ time resolved reflectivity was used to dynamically measure the extent of regrowth as a function of amorphous layer thickness for C, Si, Au and Ge beams at MeV energies incident in both channeling and random crystal directions. Results indicate that silicon displacements at the interface are responsible for the crystallisation process and cascade effects with different mass ions can have a strong influence on crystallisation rate. Buried amorphous layers are also examined and large differences in growth of front and back interfaces under channeling conditions may indicate that the first row of “amorphous” atoms at the interface may be partially aligned with the crystal rows. *(G. Azevedo, M.J. Conway, I.M. Young, J.S. Williams and A. Kinomura [ONRI, Osaka])*

Cavities in silicon have previously been shown to be very efficient trapping sites for many fast diffusing metal impurities in silicon. In the present study, neutron activation analysis, RBS/C, TEM and SIMS are used to study non-equilibrium aspects of this process in some detail. High concentrations of both Au and Cu, which initially precipitate at cavities, are found to dissolve into the bulk of the wafer extremely slowly. This phenomenon is thought to be related to the system seeking a lowest free energy state of completely filled cavities, in the absence of silicon interstitials which would allow the metal to be released. In another experiment, Au and Cu are found to be excellent detectors for open volume defects and will always decorate such defects in preference to interstitial based clusters and loops. In contrast, Fe tends to decorate both vacancy and interstitial based defects. There has been some controversy recently as to the nature of so-called Rp/2 defects in silicon. These are defects that appear up to about half the projected ion range in ion irradiated silicon after annealing. They are often sites for metal trapping. In a recent set of experiments, we studied such defects using TEM and RBS/C and also gold as a selective detector for vacancy-type defects. Results have clearly shown that vacancy clusters are the origin of Rp/2 defects. Furthermore, the numbers of vacancies contributing to such clusters after annealing is about 1% of the excess vacancies generated at depths less than Rp/2 during ion irradiation. *(J.S. Williams, M.J. Conway, I.M. Young, J. Wong-Leung, M. Petravic, B. Stritzker, B.C. Williams and A. Kinomura [ONRI, Osaka])*

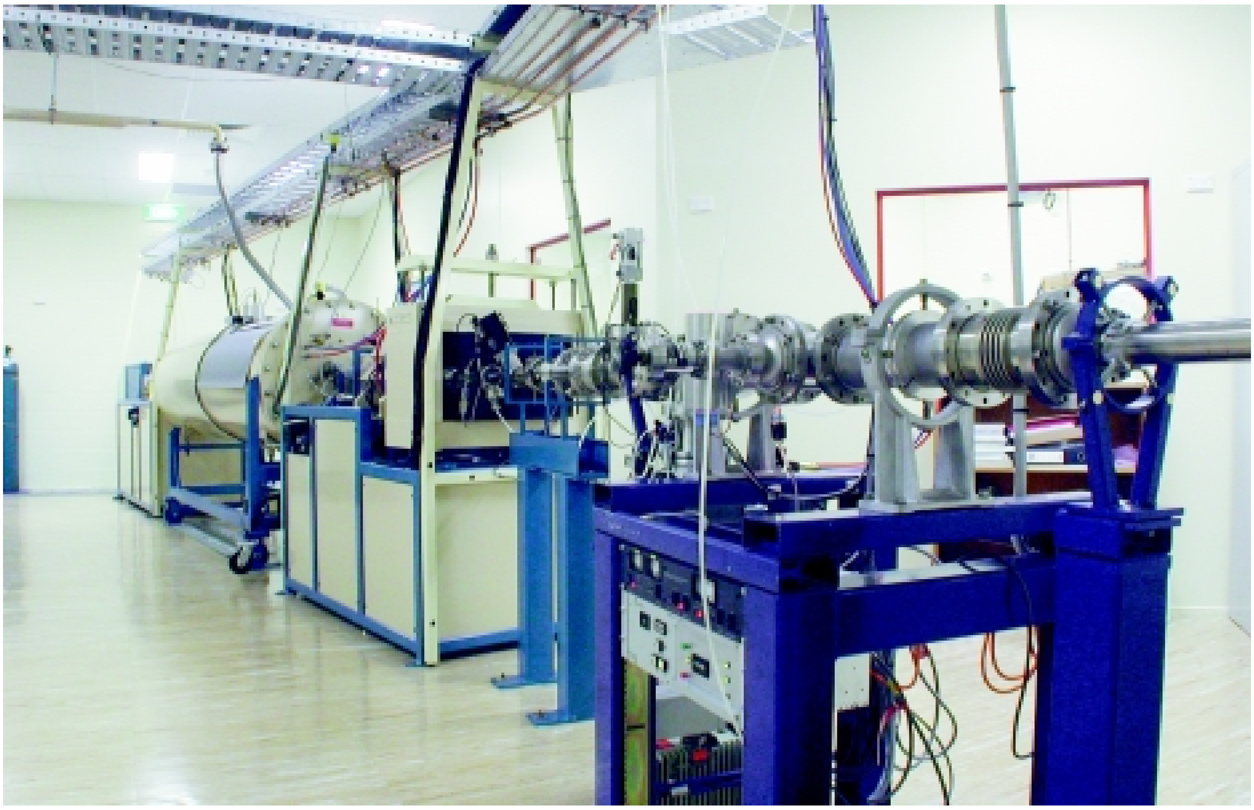
Wurtzite GaN films exposed to ion bombardment have been studied by RBS/C, TEM, atomic force microscopy (AFM), scanning electron microscopy, environmental scanning electron microscopy, cathodoluminescence, nanoindentation, and IV and Hall measurements. In particular, the following aspects of ion beam processes in GaN have been studied: (i) the influence of implant conditions on the damage build-up behaviour, (ii) strong dynamic annealing and its consequences, (iii) defect types, (iv) amorphisation, (v) preferential loss of nitrogen, (vi) ion-beam-induced porosity and material dissociation, (vii) anomalous surface erosion during ion bombardment at elevated temperatures, (viii) the effect of implantation disorder on mechanical properties, (ix) chemical effects due to high concentration of implanted species, (x) problems with annealing of amorphous GaN, (xi) ion-beam-induced reconstruction of amorphous GaN, (xii) the effect of implantation-produced defects on luminescence and (xiii) implantation studies of the chemical origin of yellow luminescence. Compared with other compound semiconductors such as GaAs and InP, GaN has been found to exhibit some extreme behaviour and property changes under ion irradiation. *(S.O. Kucheyev, J.S. Williams, C. Jagadish, J. Bradby, H. Boudinov, M. Toth, M.R. Phillips [University of Technology, Sydney] and G. Li [LEDEX])*

Ion implantation into InP is being studied for shortening the carrier lifetimes for ultrafast photodetector applicatons. It was found that annealing at 600°C for 30s produced good mobility and low (ps) lifetimes but low resistivity (n-type). It was found that, as the implant ion mass was increased, the carrier lifetime decreased. Work is being carried out to ascertain what is the role of ion mass, ion group (group III or group V), implant dose, implant temperature and annealing temperature on the structural, electrical and optical properties of semi-insulating InP. Further implants were done on p-type InP epilayers to increase the resistivity while maintaining good mobility and low carrier lifetime. Low carrier lifetimes were also observed in these epilayers and Hall effect measurements indicated that it was possible to compensate p-type InP by ion implantation at a critical dose which corresponded to the highest sheet resistance. *(C. Carmody, H. Boudinov, H.H. Tan, C. Jagadish, M.J. Lederer [LPC], V. Kolev [LPC], B. Luther-Davies [LPC]; L.V. Dao and M. Gal [UNSW])*

The electrical isolation of InP, GaN and AlGaAs conductive layers by ion irradiation was studied *in-situ* during irradiation, with different ions as a function of the irradiation dose. Lower threshold dose is needed to isolate p-type InP, compared with n-type InP with a similar free carrier concentration. A particular defect, with a characteristic annealing temperature of 200–300°C, is the major cause for the trapping of electrons. Irrespective of the irradiated dose, the thermal stability of implant-isolated n-type InP is limited to temperatures lower than 200°C, while for p-type the temperature is as high as 500°C. The sheet resistance of n-type GaN layers isolated by MeV ion irradiation increases up to 1-2x10^{11} Ω/sq during ion irradiation, and the threshold dose depends linearly on initial free electron concentration and reciprocally on the number of atomic displacements. The evolution of the sheet resistance of conductive AlGaAs layers during proton irradiation and the stability of the so-formed isolation during post-irradiation annealing were studied. To achieve maximum thermal stability (450°C for p-type and 600°C for n-type AlGaAs), the ratio between irradiated dose and threshold dose should be at least 8. This study may, as a result, have significant technological implications for choosing implant conditions necessary for an effective electrical isolation of real devices. *(H. Boudinov, T. van Lippen, S.O. Kucheyev, H.H. Tan and C. Jagadish)*

Materials Preparation, Analysis and Characterisation

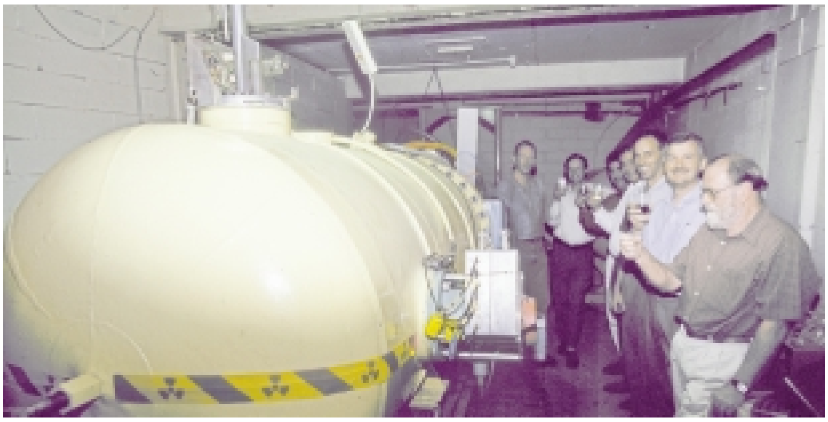
Stoichiometric and overstoichiometric silicon nitrides can be formed by bombardment of Si with low energy nitrogen ions in



The newly installed diagnostic accelerator

Research Accomplishments (EME)

Staff members toast the old Van de Graaff as it is retired after 37 years service



the SIMS apparatus. Below the critical impact angle for nitride formation, the signal of positive secondary nitrogen ions shows strong oscillations during the initial stages of nitride formation (before establishment of a dynamic equilibrium). We have studied in detail the dynamics of this transient region and found an analogy between the signal oscillations and the response of an electrical circuit made up of a resistor, a capacitor and an inductor. This analogy enabled us to model the experimental results by the response of a dissipative electrical oscillatory circuit. *(M. Petravic and P.N.K. Deenapanray)*

Ion beam mixing during SIMS profiling deteriorates the resolution of sharp interfaces or abrupt changes in impurity distributions. Buried delta-doped layers are shown to be very useful systems for setting up the standard procedures to evaluate the SIMS depth resolution. We have used GaAs delta-doped multilayers in Si, grown by the UHV ion-beam-sputter-deposition technique, as the reference material. We have shown that, in this case, the SIMS depth resolution for oxygen and cesium ion-bombardment can be estimated quite well with an analytical expression based on a double exponential (for the leading and the trailing edge of the impurity profile) and a Gaussian-like rounded top. We have continued to study the influence of surface roughening on SIMS depth resolution in Si. AFM was used to examine the roughening of SIMS craters obtained by oxygen- and nitrogen-beam bombardment at different angles of incidence. A correlation has been found between the critical angle for oxide formation and the enhanced roughening of the crater bottoms. The enhanced roughening in this transient region between Si and SiO_2 is most probably caused by the nonuniform coverage of a Si surface by oxides and the different sputtering rates of Si and its oxides. *(M. Petravic, P.N.K. Deenapanray and D.W. Moon [KRISS, Korea])*

We have continued the study of selective photo-stimulated desorption from hydrogenated GaAs surfaces using the high-resolution photoemission from the GaAs (100) surface around Ga 3d and As 3d levels as a function of hydrogen exposure. In this study we used photons in the 40-160 eV range from the beam-line 08A LSGM at the Synchrotron Radiation Research Center in Hsinchu, Taiwan. The polar GaAs (100) surface was As-terminated and, for the low exposure ($1x10^4$ L of H_2), hydrogen atoms bond preferentially to As as demonstrated by the chemical shift of As 3d levels (no shift of Ga 3d levels observed for this low exposure). For the higher exposures (above $5x10^4$ L of H_2), hydrogen saturates the As dangling bonds, breaks the As dimer bonds and finally causes desorption of As as AsH_3, transforming the surface into a Ga-rich surface. In agreement with this picture, the photoemission around the Ga 3d edge clearly shows the shift in the Ga peak and finally the dominance of the Ga signal related to the pure Ga on the surface, over the signal related to the GaAs. *(M. Petravic, P.N.K. Deenapanray and J-M. Chen [SRRC, Taiwan])*

Gas ionisation detectors were originally developed for nuclear physics research but have more recently found use in nuclear techniques of analysis including heavy ion elastic recoil detection. However, the response of such detectors has been shown to depend on the mass and energy of the detected ion, with the measured pulse amplitude decreasing with increasing atomic number Z, for a given ion energy. Measurements were performed for a wide range of ion species and energies and various techniques used to estimate the contribution of energy loss of the ions in the detector window, as well as the energy lost by the ions during elastic collisions within the gas volume. These have shown for the first time that there is a significant residual pulse height deficit after accounting for such effects. The origin of this residual effect is currently being studied. *(T.D.M. Weijers, T.R. Ophel [NP], H. Timmers and R.G. Elliman).*

In a parallel study, the response of silicon surface-barrier detectors to heavy ions was also examined. We were able to show for the first time that the effective energy required to produce a detectable electron-hole pair first decreases and then increases with increasing ion mass, so that a pulse height surplus was recorded for masses up to 80 amu and a pulse height deficit for higher masses. This has important implications for precision measurements using surface barrier detectors and further studies of the underlying mechanisms are in progress. *(J.A. Davies, T.D.M. Weijers, T.R. Ophel [NP], H. Timmers and R.G. Elliman)*

Accurate energy loss and straggling data are required for quantitative ion beam analysis. Unfortunately, the accuracy of such data for high-energy heavy ions is limited to ±20%, imposing limits on the accuracy of techniques such as heavy ion elastic recoil analysis and heavy-ion backscattering spectrometry. In a collaborative study with the University of Lund and the University of Newcastle, measurements of the stopping power and straggling of a range of heavy ions have been undertaken for energies around 1 MeV/amu. *(H. Whitlow [University of Lund] D.J. O'Connor [University of Newcastle] H. Timmers, T.D.M. Weijers and R.G. Elliman)*

Heavy-ion elastic recoil detection can provide quantitative analysis, including depth profiles, of a broad range of elements, including H. This has led to several new collaborative studies involving characterisation of thin film materials. These include: a) the continuation of a collaborative project with the Plasma Research Laboratories on the characterisation of doped silica films for use in integrated optics applications (*T.D.M. Weijers, K. Gaff [Plasma Physics], H. Timmers and R.G. Elliman*); b) a project with the University of New England involving quantitative compositional analysis of plasma-nitrided stainless steel (*M.P. Fewell [University of New England], H. Timmers, T.D.M. Weijers and R.G. Elliman*); c) a study with Macquarie University on the analysis of GaN films grown on (100) silicon and (0001) sapphire by plasma-assisted laser-induced vapour deposition (*K.S.A. Butcher [Macquarie University], H. Timmers, T.D.M. Weijers and R.G. Elliman*); d) a project with the Korea Research Institute of Standards and Science (KRISS) on the measurement of ultra-thin oxide layers (*D-W. Moon [KRISS, Korea], H. Timmers, T.D.M Weijers and R.G. Elliman*) and e) a project with McMaster University on the analysis of thin oxy-nitride layers deposited by ECR-PECVD. *(J.A. Davies [McMaster], H. Whitlow [University of Lund], J. Uribasterra [University of Lund], T.D.M. Weijers, H. Timmers and R.G. Elliman)* .

Microindentation studies have been undertaken on a range of semiconductors to correlate mechanical properties with structural changes, including phase transformations. TEM, AFM and microRaman techniques have been used to characterise the indents. In Si the complete sequence of deformation processes has been observed for the first time. Prior to catastrophic plastic deformation, both slip and a small volume of Si transformed to a plastic, metallic phase have been observed. In compound semiconductors the major mode of deformation is slip rather than phase transformation. Deformation mechanisms involving both phase transformation and slip have been proposed. *(J. Bradby, J.S. Williams, J.L. Wong-Leung, M. Swain [University of Sydney], P. Munroe [UNSW] and J. Fitz Gerald [RSES])*

The most exciting result obtained this year in the mechanochemistry area is high yield boron nitride nanotube production by a novel reactive ball milling method. This result has clearly demonstrated that the reactive ball milling process could become a large-scale synthesis method for BN nanotubes. To date, high quantities of pure BN nanotubes have not been produced with other production methods. Because of the difficulties in producing BN nanotube samples, research on properties and applications of BN nanotubes is much behind carbon nanotubes. We are currently addressing this situation. Multi-walled carbon nanotubes have also been produced by ball milling of graphite powder at room temperature and subsequent thermal annealing at 1400°C. The mechanical treatment produces a disordered and microporous structure, which provides nucleation sites for nanotubes as well as free carbon atoms. Multi-walled carbon nanotubes appear to grow from single-wall nanotube embryos via growth of the (002) layers during thermal annealing. *(Y. Chen, M.J. Conway, J. Fitz Gerald [RSES], J.S. Williams and L. Chadderton [AMPL])*

Complex, mixed oxides are important for a number of applications, including fuel cells. Strontium-iron oxide is one such material which can exist in a number of oxidation states. It is crucial in such materials to understand the relationship between stoichiometry and structure. In this study, X-ray and neutron diffraction, thermal analysis (including thermogravimetry) and Mossbauer spectroscopy have been used for the first time to detail the structure and local atomic environment over the entire

The new MOCVD reactor eager to begin its work composition range. Models have been proposed to explain the results. *(M. Schmidt, S.J. Campbell [ADFA] and J.S. Williams)*

A remarkably simple process for the formation of bulk quantities of submicron single crystals of hard materials such WC, TiB_2, TiC, TiN and TaC directly from mineral concentrates has been investigated and shows considerable promise for commercialisation. Separation of tantalum from niobium is typically performed after dissolution of a mineral concentrate into hot, concentrated hydrofluoric acid which is extremely hazardous. Extended premilling of the mineral concentrate has resulted in the rate of dissolution increasing 4500 fold compared with unmilled powder thereby allowing either less aggressive conditions to be used or a greater throughput in an existing plant. *(N.J. Welham)*

Semiconductor nano-particles of germanium have been made by milling elemental germanium in an inert matrix which is then chemically removed. Raman spectroscopy of these particles show quantum confinement with peak shifts of 7 cm^{-1} measured. Previous studies have reported shifts <4 cm^{-1} indicating that these particles are substantially smaller than those produced by other methods. Preliminary work has shown that GaAs can readily be reduced to isolated single crystal cubes with edges <500 nm. *(N.J. Welham, C. Jagadish and M. Gal [UNSW])*

MOCVD Growth of III-V Compound Semiconductors

A new MOCVD reactor was purchased from Aixtron AG, Germany and installed in June this year. The table below summarises the results achieved from single layer growths to date.

A variety of multi-layered and optoelectronic device structures were grown including AlGaAs, InGaAs on GaAs and InGaAs on InP, quantum well, laser and photodetector structures, GaAs-AlGaAs distributed Bragg reflectors and semiconductor saturable absorber mirrors at 946 and 1064 nm. In particular, quaternary InGaAsP material grown on InP has shown significant improvement with the commissioning of the new reactor. Lattice matching was achieved to less than 100 ppm with excellent uniformity. This project is of particular importance as it allows access to optical material/devices in the telecommunication wavelengths of 1.3 and 1.55 µm. Work in the design and growth of laser diodes in this wavelength regime is now progressing. *(H.H. Tan, P. Lever, L. Fu, Q. Gao, M. Buda and C. Jagadish)*

Delta doping of InP-InGaAs with Si, Zn and C is being investigated. This study aims to identify the mechanism of incorporation of a very thin layer of dopants during epitaxial growth. Various parameters are investigated, such as growth temperature, pre- and post-purge times and growth pressure. It was found that $>1\times10^{19}$ cm^{-3} of peak Si concentration could be incorporated into InP with a narrow profile depending on the growth sequence. The study on Zn delta doping is even more exciting due to a fundamental limit in the incorporation of this dopant ($\sim3\times10^{18}$ cm^{-3}) in bulk InP. *(Q. Gao, H.H. Tan and C. Jagadish)*

Impurity-free interdiffusion of GaAs/AlGaAs and InGaAs/InP quantum wells has been studied using a number of capping layers, such as spin on glass, oxides of As and Ga and silica deposited by plasma enhanced chemical vapour deposition (PECVD). The influence of stress of PECVD silica on AlGaAs/GaAs heterostructures has been shown to be a key parameter controlling the interdiffusion mechanism. In the InGaAs/InP quantum wells, it was found that, at low annealing temperatures, intermixing was suppressed in capped samples as compared to purely thermal intermixing. The mechanism of interdiffusion in this material system is quite complex as it depends significantly on the quality (and the lattice matching) of the starting material. For spin-on-glass cap layers Fourier transform infrared spectroscopy, spectroscopic ellipsometry and chemical etching, together with the photoluminescence (PL) measurement results, have shown a direct correlation between the film quality and quantum-well intermixing. Doped (As, P, Ga) spin-on-glass was also used for interdiffusion studies. A Ga-doped cap has been found to suppress interdiffusion while a P-doped cap slightly enhances the interdiffusion. Although oxides of Ga and As can be formed by anodic oxidation, they are not satisfactory as capping layers. Deep level transient spectroscopy has been used to study the electron traps created in rapid thermally annealed (RTA) SiO_2-capped n-type GaAs epitaxial layers. The deep levels are related to the increase in the As:Ga ratio in the GaAs layer close to the encapsulant/GaAs interface due to the outdiffusion of Ga atoms in the SiO_2 layer during RTA. Isochronal annealing studies have shown that the dominant electron traps are removed between 500-600°C. *(P.N.K. Deenapanray, C. Carmody, L. Fu, R. van der Heijden, M. Petravic, H.H. Tan, C. Jagadish; L.V. Dao and M. Gal [UNSW])*

The table summarises the results achieved from single layer growths to date

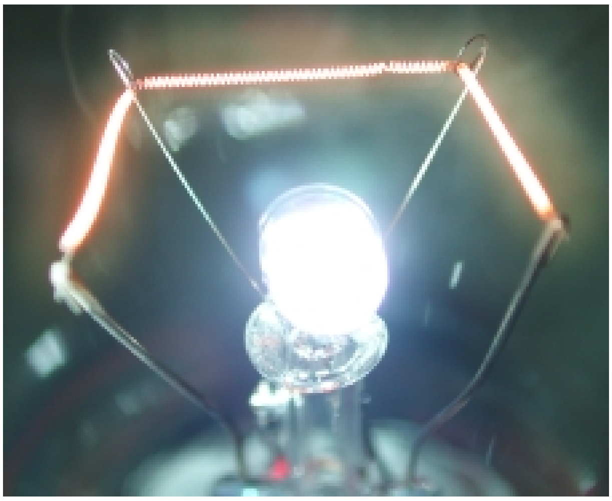
Material System	Properties	Values achieved
GaAs	• Mobility at 77K • Background doping	73 700 cm^2/Vs 2.5×10^{14} cm^{-3}
$Al_{0.3}Ga_{0.7}As$	• Background doping • PL FWHM at 300K • PL FWHM within wafer • PL peak within wafer (300K)	8.5×10^{15} cm^{-3} 30 meV σ ~0.7 nm σ ~0.2 nm
InP	• Background doping • Mobility at 77K	$1.7\times10^{15}cm^{-3}$ 204 000 cm^2/Vs
$In_{0.53}Ga_{0.47}As$ (on InP)	• Background doping • Mobility at 77K • Lattice mismatch	$2.2\times10^{15}cm^{-3}$ 120 000 cm^2/Vs σ ~1.2×10^{-4}
InGaAsP (on InP) **λ = 1300 nm ± 20 nm**	• Within wafer • Wafer to wafer	σ ~2.6 nm σ ~0.9 nm
InGaAsP (on InP) **λ = 1550 nm ± 20 nm**	• Within wafer • Wafer to wafer	σ ~2.8 nm σ ~1.3 nm

Electronic and Optoelectronic Devices

In the area of optoelectronic devices, proton implantation has been used to fine tune the emission wavelengths of quantum well lasers. The implantation and annealing conditions were based on our previous work of implantation intermixing of InGaAs/GaAs and InGaAs/AlGaAs quantum wells, where large photoluminescence (PL) energy shifts were observed in both materials. However, in InGaAs/AlGaAs samples larger PL energy shifts and also better recovery of PL intensities were obtained, which was ascribed to dynamic annealing effects in AlGaAs during implantation. Based on these results, InGaAs/AlGaAs quantum-well lasers were fabricated and up to 49.3 nm emission wavelength shift was observed in the proton-implanted lasers with no significant degradation in the main device characteristics. *(L. Fu, H.H. Tan and C. Jagadish)*

Further application of implantation induced intermixing was in the area of quantum well infrared photodetectors (QWIPs). By modifying the bandgap of the quantum wells, the detection wavelength of QWIPs could be fine tuned, leading to the integration of multi-colour QWIPs. A very efficient and effective high energy implantation scheme was employed to achieve a uniform intermixing in the QWIPs structure, leading not only to large shifts in spectral wavelength, but also to modified spectral linewidth, which is in good agreement with the theoretical calculation reported in the literature. By further performing a two-step implant-anneal sequence to optimise the single high energy implant scheme, the device performance was further improved, showing the promising application of this method in realising multi-colour QWIPs. *(L. Fu, H.H. Tan and C. Jagadish)*

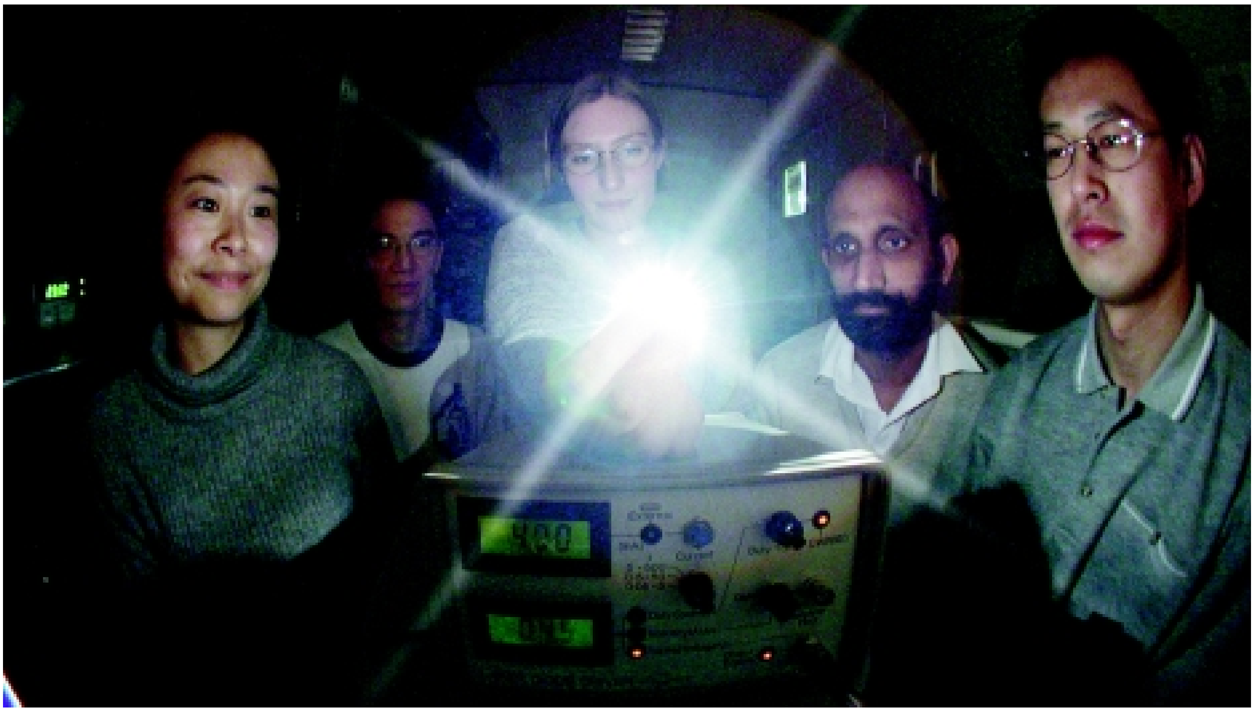
Vertical cavity surface emitting lasers (VCSELs) are promising in free space optical interconnect applications. In particular steerable VCSELs are of significant interest as they allow the fabrication of dynamically reconfigurable free space interconnects. We have fabricated an electrically steerable laser based on wide aperture VCSELs exhibiting low cross talk and large steering range by fine control of the device aperture.



Old technology, new technology. A white LED sits inside the filament of a conventional light bulb

Transient measurements indicate the steering behaviour is controlled by thermal lens processes in the device aperture. A dynamically reconfigurable optical switch based on this device was made with crosstalk between channels of better than 18 dB. A provisional patent was filed. *(M.I. Cohen, C. Jagadish; A.A. Allerman and K. Choquette [Sandia National Laboratory])*

Work on high power 980 nm AlGaAs quantum well lasers is progressing with in-house development of mounting the device on Cu heat sinks. Preliminary results from wafers grown in the new MOCVD reactor were very encouraging where CW kink-free power of ~270 mW was achieved for a 4 mm-wide and 2 mm-long device. Reliability testing of the device is currently being performed. This project is of great importance as this technology will be used by Acton Lasers for the manufacturing of single and multi-mode high power 980 nm lasers for optical pumping of Erbium-doped fibre amplifiers (EDFAs). *(M. Buda, L. Fu, J. Hay, H.H. Tan and C. Jagadish)*



Some members of the devices group with a high power white LED

Metal-Semiconductor-Metal (MSM) photodetectors were used to investigate the effects of self assembling monolayers on GaAs. MSM inter-digitated gold patterns were deposited on a GaAs substrate and dark current voltage measurements were performed to see if deposition of self assembling monolayers caused a reduction in the surface leakage current. No significant change was seen as compared to as-etched samples (where the surface oxide was removed). Further experiments will be performed using more sensitive equipment, since these measurements were made at the detection limits of the current equipment. Also, experiments are planned to measure the change in surface leakage current over a period of days after treatment with self-assembling monolayers. *(C. Carmody, H.H. Tan, C. Jagadish; L.V. Dao and M. Gal [UNSW]; V. Braach-Maksvytis and B. Raguse [CSIRO-TIP])*

In collaboration with the Laser Physics Centre, semiconductor saturable absorber mirrors have been designed and grown for mode-locking of solid state lasers at 1064 nm and 946 nm. Ion-implantation as a tailoring technique for these devices has been developed to achieve a very high degree of flexibility of the desired device response such as response time and modulation depth. *(H.H. Tan, C. Jagadish; M.J. Lederer, V. Kolev and B. Luther-Davies [LPC])*

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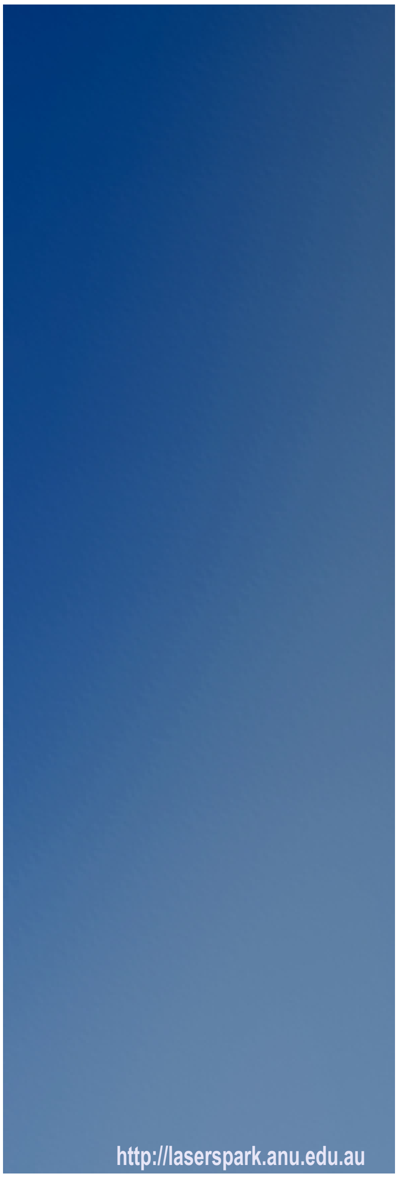


The Laser Physics Centre is engaged in laser-based research on topics spanning both fundamental and applied physics and engineering.

Research Summary

The Laser Physics Centre is engaged in laser-based research on topics spanning both fundamental and applied physics and engineering.

Much of the research of the Centre involves some aspect of materials science, such as the development of linear and nonlinear materials for photonics, or laser-based methods for the production of new materials or unusual states of matter. Almost all of the projects undertaken in the Centre involve extensive collaboration with local and overseas groups. Within the School we have strong interactions with the Department of Electronic Materials Engineering, Applied Mathematics, the Optical Sciences Centre, the Atomic and Molecular Physics Laboratories and the Plasma Research Laboratory. Outside the School we have projects with the Departments of Chemistry and Physics and Theoretical Physics at the ANU, Australian Defence Force Academy, James Cook University, University of Sydney, and overseas groups in USA, Germany, UK, Poland, France, Switzerland and Russia.

The Centre remains a strong contributor to the Australian Photonics Cooperative Research Centre in which Professor Barry Luther-Davies holds the position of Research Director and is one of the Directors of Australian Photonics Pty Ltd, the Commercial and Management agent for the Cooperative Research Centre (CRC). During 2000 we have achieved breakthroughs in low loss organically modified silicate glasses for the fabrication of planar lightwave circuits which is motivating a commercialisation activity in this area involving a new company – Redfern Polymer Optics.

Several new staff members joined the Centre during the year. Dr Anke Freydank joined the Centre to work on novel chromophores for nonlinear optics. Dr Reiner Friedrich and Dr Congji Zha joined the Centre with funding from the CRC to work on organically modified silicate glasses. Ruth Jarvis was another CRC appointee working on the fabrication of optical waveguide devices in organically modified silicate (ORMOSIL) and polymeric materials. Kristina Milas joined the Centre as Departmental Administrator replacing Lesley Elliott. Darryl Scott joined the Centre as a PhD student to work on photonic signal processing. Dr Robbie Charters resigned his CRC funded position to take up a post initially with Nortel and then with Redfern Polymer Optics but maintains strong links with the Centre. Dr John Martin left the Solid State Spectroscopy group to take a position in the Australian Bureau of Statistics. Dr Chanjiang Wei left the Centre in September and is now working in the IT industry.

Professor Byeong-Soo Bae from KAIST Korea spent a productive twelve months with the Centre working on silica-zirconia based ORMOSILs, funded by an IREX grant. Dr Abdulnassar Zakery from Shiraz University in Iran remained with the Centre until October on sabbatical leave and produced some novel results on arsenic trisulphide glasses. We continue to benefit from the expertise of Dr Alex Boiko from Electro Optic Systems Pty Ltd who produces high quality optical coatings in support of the research as well as servicing the needs of the company. Alex was the year 2000 recipient of the Australian Optical Society's Technical Optics Award for his work on innovative optical coatings.

Nonlinear Optical Materials and Structures

Our ability to study the nonlinear optical (NLO) properties of various materials has been greatly enhanced this year by the acquisition of a new RIEFP/ANU funded high-power tunable femtosecond laser system. This system, based on a Ti-sapphire regenerative amplifier and an optical parametric generator, is capable of producing high-power femtosecond duration (about 150 fs) laser pulses in a wide range of wavelengths, including the visible range as well as the technologically important ranges of 1.3-1.6 micron. When all the data collection equipment is completed, the system will be able to provide information on nonlinear optical properties of many materials such as polymers, glasses and semiconductors.

Third-order NLO Properties of Conjugated Polymers, Model Molecules and Organometallics

We have been investigating nonlinear optical properties of several different classes of organic compounds. This work has involved collaboration with groups in Australia (Dr Mark Humphrey's group at the ANU) and from overseas (e.g. groups in Jena, Germany and in Lyon, France).

Nonlinear Optical Properties of Soluble Derivatives of Poly(p-phenylene vinylene)

Third-order nonlinear optical polymers built of rigid-rod molecules are often insoluble and transmit visible light poorly. We have undertaken collaborative studies of the optical and waveguiding properties of a new soluble derivative of poly(p-phenylenevinylene) (PPV): a π-conjugated polymer poly[biphenyl-4,4'-diyl-1,2-di(4-fluorophenyl)vinylene], (DFP-PDPV) synthesised in the laboratory of Professor Hans Hörhold and Dr Regina Stockmann from the Institut für Organische Chemie und Makromolekulare Chemie, Friedrich-Schiller-Universität in Jena, Germany.

The linear optical properties of thin films – birefringence and dispersion of refractive indices were measured in the wavelength range from 476.5 nm to 1.55 µm; absorption spectra in the range 200-3200 nm; and waveguide propagation losses at 632.8 nm, 810 nm and 1064 nm. The losses decreased at longer wavelengths reaching the level of 1 dB/cm at 1.06 µm. The waveguiding properties of DFP-PDPV films depended on the solvents used in processing of the polymer. The modulus of nonlinear refractive index $|n_2|$ in the range (0.9-1.5) $\times 10^{-14}$ cm^2/W was measured in films at 800 nm using a femtosecond degenerate four wave mixing (DFWM) technique. These studies supplemented the results of nonlinear optical studies of the polymer in solution using the Z-scan technique. *(A. Samoc, M. Samoc and B. Luther-Davies)*

Third-order Nonlinear Optical Properties of Soluble Conjugated Polyenes

The NLO properties of soluble polyenes were studied in the collaboration with Dr Chantal Andraud and Dr Thierry Brotin, Stereochimie et Interactions Moleculaires École Normale Superieure de Lyon, France.

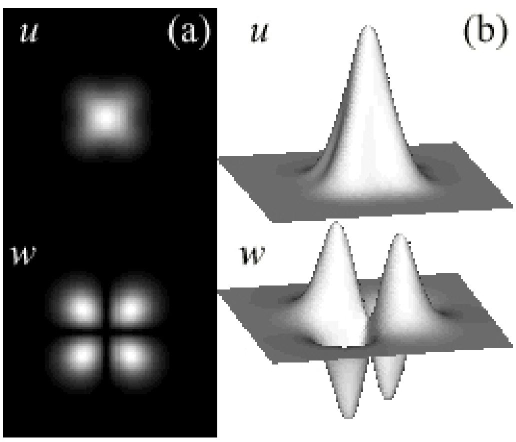
The technique of closed and open aperture Z-scan at 800 nm was used to investigate third-order nonlinear optical properties of 5 symmetric polyene molecules, symmetric polyenovanillins possessing a sequence of conjugated double bonds: (-CH=CH-)n, for n=3-8, terminated with phenyl groups substituted with solubilising agents. Absorption spectra showed strong shifts to longer wavelengths with increasing number of double bonds. Z-scan measurements in solutions showed strong variations of the nonlinear refractive index and third-order hyperpolarisabilities. The two-photon absorption increased with increasing number of double bonds. The real part of the nonlinearity showed a solvent dependence and saturation properties for femtosecond laser pulses. The results emphasise the importance of dispersion for nonlinear optical properties of conjugated molecules. Work is in progress to explain the origin of this effect. *(A. Samoc, M. Samoc, B. Luther-Davies and M.G. Humphrey [Chemistry, The Faculties])*

Soliton Physics

Our work on optical spatial solitons, which is now partially supported by a grant from the Performance and Productivity Fund, continues to attract strong international interest. Two aspects of our research will be featured in the Optical Society of America's annual review *Optics 2000*, one on the *Nonlinear Aharonov-Bohm Effect for Optical Vortices*, and the other on *Molecules of Light: Dipole-mode Vector Solitons*. The work of the group was further recognised by an invitation to Professor Barry Luther-Davies to lecture at a NATO Summer School on Spatial Solitons in Swinoujscie, Poland in October.

Our research is carried out in collaboration with theoreticians of the Optical Science Centre and many overseas researchers. A particularly notable development this year has been the observation of multi-pole vector solitons. A dipole mode vector soliton is composed of a Hermite-Gaussian HG_{01} mode co-propagating with a fundamental soliton. Our theoretical work and experimental studies have demonstrated the remarkable stability of these vector solitons which can even survive collisions which impart angular momentum to the dipole component. We have lately expanded the concept to demonstrate the formation of a robust quadrupole mode vector beam, whilst numerical studies have shown that even higher order structures such as octopoles can also exist.

We have extended our studies of partially coherent solitons and developed a unified model for such structures in a logarithmic nonlinear medium which shows that complex internal dynamics can exist as is anticipated for the general class of saturating nonlinear media. *(W. Krolikowski, G. McCarthy, M. Geisser, D. Edmundson; E. Ostrovskaya and Y. Kivshar, [OSC]; C. Denz and C. Weilnau [Darmstadt] and O. Bang [TU Denmark])*



The field and intensity structure of a quadrupole vector soliton. Upper images show the fundamental soliton which co-propagates with the quadrupole structure shown in the lower images.

Photonic Materials and Devices

Organic Waveguides for Photonics

Polymers or organically modified silicate glasses (ORMOSILs) offer many advantages for the production of thin film optical waveguides, such as low processing temperatures, simple processing techniques, and compatibility with both organic and inorganic dopants. The main difficulty has proved to be the production of material with sufficiently low losses in the important 1.3 μm and 1.55 μm telecommunications windows for practical purposes.

In the past twelve months, we have investigated the processing and determined the important optical properties of several ORMOSIL systems. This has included the methacrylate silica-zirconia system, the methacrylate/phenyl/silica system, a two component fluorinated arylsilane system, as well as some novel phenyl/vinyl/silica and phenyl/methacrylate/silica systems capable of reduced optical losses. We have made extensive measurements of the refractive index and its tunability; the optical losses and photosensitivity that can be obtained in these glasses, along with their film forming properties and processability. The main characteristics of some of these polymers are low losses in the NIR region (0.2 dB/cm at 1310 nm and 0.6 dB/cm at 1550 nm), very good reproducibility and a tunable refractive index.

We have continued to refine our devices production facilities involving UV laser direct writing and have used this to demonstrate low-power consumption thermo-optic space switches using a novel waveguide design using refractive index up and down tapers. *(R. Charters, A. Samoc, M. Samoc, B. Luther-Davies, C. Zha, R. Friedrich, G. Atkins [U. of Sydney] and B. Bae [KAIST, Korea])*

Polymer Fibre for Voltage Sensing

We continued fabrication and characterisation of polymer fibres containing a longitudinally poled electro-optic core for use as a fibre optic voltage sensor. The project is supported by ABB and Transgrid. During this year there were two main aims: to create a single mode optical fibre with a core containing the electro-optic chromophore Disperse Red 1, and secondly, to synthesise the MTPV-ORSO chromophore which was designed to provide low optical loss for the fibre in the region of maximum transparency for PMMA around 650 nm.

We have spent a lot of time fabricating fibre preforms of poly(methylmethacrylate) (PMMA) doped with the side chain electro-optic chromophore, PMMA-Disperse Red 1. We have studied the influence of the dopant on parameters such as the glass transition temperature of the polymer, and its refractive index. A major challenge has proved to be obtaining preforms where the core and cladding can be drawn into fibre at the same temperature. The PMMA based polymer fibre has been pulled in the drawing tower constructed at the Laser Physics Centre.

The synthesis of the MTPV-ORSO chromophore has proved quite challenging since deficiencies were identified in the procedure developed for us by Dr Ricky Wong some years ago. A poly(methyl methacrylate) co-polymer with a phenylene-vinylene side group has now been successfully synthesised. The key step to the successful production was the introduction of an asymmetric centre in the molecule. The newly developed synthesis contains 12 reaction steps, including the monomer synthesis and the co-polymerisation. All intermediates are spectroscopically characterised. The chromophore bears a glycol substituent on one side and an n-decyl chain on the other side.

For guest-host systems of a chromophore in a polymeric matrix, a sufficient solubility of the polymer is necessary. It was found that the solubility of co-polymer is not high enough to incorporate it efficiently into a methacrylic matrix for producing a preform.

To overcome the problem of the solubility, the shape of the alkyl substituent was changed from a n-decyl chain towards a branched alkyl chain. The new synthesis includes 14 reaction steps including the synthesis of the branched alkyl thiol which is then converted by nucleophilic substitution into a 4-(1-ethyl-butylthio) benzaldehyde. The newly developed chromophore shows a highly improved solubility in common organic solvents and in methyl methacrylate host solution. The new monomer offers the possibility of incorporating the optically active compound into the polymeric matrix by chemical bonding and delivers a material where the chemical and physical properties of the active chromophore are homogenously distributed. *(A. Freydank, B. Luther-Davies, A. Samoc, M. Samoc, R.M. Krolikowska, C. McLeod, T. Martin, J. Bottega and I. McRae)*

Laser Matter Interaction Physics

Pulsed Laser Deposition of Chalcogenide Glasses

Chalcogenide glasses show a wide variety of photo-induced effects as a result of illumination. These effects can be used to fabricate diffractive as well as waveguide structures. This year, we have applied our Ultra-Fast Laser Deposition technique to formation of As-S and Ge-As-Se chalcogenide glass films for waveguide applications. Up to now, vacuum evaporated films have been used to fabricate waveguides in As-S-Se system of glasses and waveguide losses have been relatively high.

Our As_2S_3 film depositions were performed using second harmonic of a mode-locked Coherent Antares Nd:YAG laser. Waveguides were written into the films using 514 nm radiation from an Argon ion laser. The results demonstrated that Ultra-fast PLD can be used to successfully fabricate low loss waveguide films of chalcogenide glasses. The films were highly photosensitive and losses as low as 0.2 dB/cm were measured at 1550 nm.

An interesting feature of chalcogenide materials is their relatively high third-order optical nonlinearity. We have investigated the third-order NLO properties of thin films of chalcogenides using the techniques of Z-scan and degenerate four-wave mixing. The nonlinear refractive index (n_2) has been determined with femtosecond laser pulses from an 800 nm amplified system as well as at several wavelengths obtained from the new optical parametric oscillator. *(A.V. Rode, A. Zakery [U. Shiraz], M. Samoc and B. Luther-Davies)*

Nonlinear Optical Effects at Gallium/Silica Interface

We have performed the first experimental study of light-induced reflectivity changes at an α-gallium/silica interface irradiated by femtosecond and picosecond duration laser pulses. The analysis shows that the laser-target interaction proceeds in non-equilibrium conditions. The sharp rise of the reflectivity in the first ~2 ps follows the cooling of the electron component of the non-equilibrium solid-state plasma heated by the laser pulse. The increase of reflectivity from the value of ~60%, typical for crystalline α-Ga, to 70-75% in ~2 ps has been measured by the pump-probe technique using a Ti-Sapphire laser (150 fs, 800 nm). After the initial 2-ps rise the reflectivity approaches the value characteristic for liquid Ga of ~85% in more than 100 ps.

The fundamental reasons behind the rapid reflectivity rise of gallium films have been considered in detail. A self-consistent treatment of laser absorption, electron heating and non equilibrium material transformation shows that the transient optical and thermal properties of the laser excited target are dominated by the temperature (time) dependent electron-phonon interaction.

The thermalisation time in the film is in the order of picoseconds, which is much longer than the laser pulse duration of 150 fs. Thus, the unusual situation arises: the electron sub-system is responding to the action of the external laser field on the femtosecond time scale, and the electron energy and number density increases affecting the optical properties of the Ga-layer, while the ions remain at the positions of the initial crystalline a-Ga. The optical response of the hot degenerated electron gas is the same as a response of hot liquid gallium in spite of the fact that the ions are still in the highly anisotropic positions of α-Ga. Therefore, one can not consider this transient state of matter as a liquid in the equilibrium thermodynamic sense, and the phase transition to that state as a melting process. *(A.V. Rode, E.G. Gamaly, M. Samoc and B. Luther-Davies)*

Femtosecond Laser Ablation

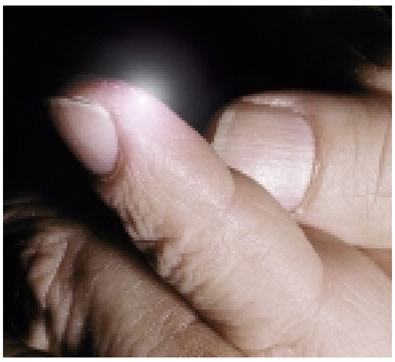
The mechanism of ablation of solids by intense femtosecond laser pulses has been considered in detail. The regime is characterised by laser intensity in the range ~ 10^{13} – 10^{14} W/cm^2 and the pulse duration shorter than the plasma expansion time, the heat conduction time, and the electron-to-ion energy transfer time. It is shown that at the high intensities when the ionisation of the target material is completed before the pulse end, the ablation mechanism appears to be common for metals and dielectrics. The physics of this new regime of ablation comprises the ion acceleration in the electrostatic field of charge separation created by energetic electrons escaping from the target. The formulae of ablation thresholds and ablation rates for metals and dielectrics, combining the laser and target parameters, are derived and compared to the experimental data. The calculated dependence of the ablation thresholds on the pulse duration is in agreement with the experimental data in a femtosecond range, and it is linked up to the dependence for nanosecond pulses. In this new regime, the threshold fluence is almost independent of the pulse duration, and the material evaporation rate is much higher than in the long pulse interaction regime.

We performed preliminary experiments on femtosecond laser ablation of dielectrics, including chalcogenide glasses. The experimental results are currently under investigation. *(E.G. Gamaly, A.V. Rode and B. Luther-Davies)*

Ultrafast Semiconductor Spectroscopy – Semiconductor Saturable Absorbers

In collaboration with EME we have continued our work on design, manufacture and characterisation of semiconductor saturable absorbers. Recent successes were the semiconductor saturable absorber mirrors (SESAMs) designed for solid-state laser mode-locking at 1064 nm and 946 nm. These proved to be of superior quality, thanks to the new Metal Organic Chemical Vapor Deposition facility at EME. We are also currently working on the femtosecond differential reflectivity characterisation of ion-implanted InP. Furthermore, design of ultra broadband SESAMs, as well as devices for all-optical switching and wavelength conversion at the communications wavelengths (i. e. 1.3 µm and 1.55 µm) are being pursued. In collaboration with the group of Professor Ursula Keller (ETH Zürich) we are investigating Beryllium doping of ion-implanted GaAs as a promising method to increase the nonlinear modulation of ultrafast ion-implanted GaAs devices. *(M. Lederer, V. Kolev, B. Luther-Davies; H. Tan, C. Carmody, C. Jagadish [EME]; M. Haim and U. Keller [ETH Zürich])*

Dr Andrei Rode demonstrates the surgical applications of high power femtosecond lasers on his own finger. Those crazy Russians!



Dr Matt Sellars of the Solid State Laser Spectroscopy group, delivers a gripping Founder's Day yarn about the one that got away (above). Back in the Lab, Matt's ultra high resolution laser (below)

Passively Mode-locked Ultrashort Pulse Solid-state Lasers

We have developed a picosecond Nd:YVO_4 laser, passively mode-locked by a semiconductor saturable absorber mirror (SESAM). The laser will be packaged by Electro Optic Systems Pty Ltd and is intended for use in satellite laser ranging systems of this company. Other picosecond SESAM mode-locked lasers demonstrated were Nd:YAG and Nd:YLF, whilst materials such as Nd:KGW are currently under investigation. Broadband ZnSe/MgF_2 output coupling mirrors have been fabricated using electron beam evaporation. These have been a key component in a recent experiment showing 5 femtosecond laser pulses generated in a Kerr-lens mode-locked Ti:sapphire laser (in collaboration with University of Karlsruhe, Germany). Very low repetition rate (<15 MHz) SESAM mode-locked high power diode pumped Nd:YVO_4 and Nd:YAG lasers are currently under development. Their aim is to provide 1064 nm and 946 nm pulses for use in ultrafast laser ablation experiments. *(M. Lederer, V. Kolev, A. Boiko and B. Luther-Davies)*

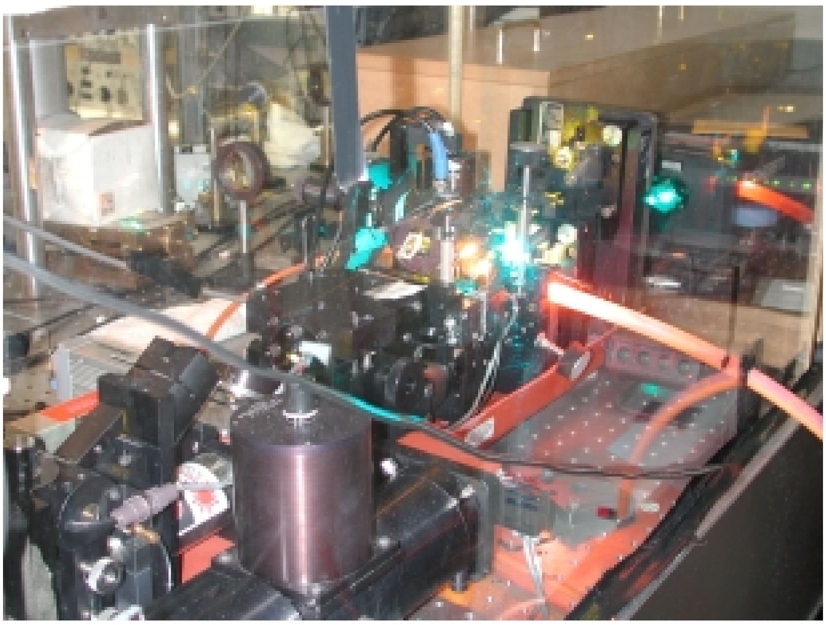
Solid State Laser Spectroscopy

There are two major research programs within the Solid State Laser Spectroscopy Group. Both involve studies of quantum coherence; one in the visible and one in the radio frequency region of the spectrum. The program at visible wavelengths deals with rare earth ions in crystals which give the narrowest optical line widths and the longest dephasing times of any transition in a solid. The studies have benefited from the development of a laser with a stability better than the optical line widths. The development of this laser has given us an advantage over other research laboratories and has enabled us to develop new spectroscopic techniques and introduce aspects of optical processing. In the case of the radio frequency studies, we capitalise on the unique characteristics of a colour centre in diamond where spin transitions in the electronic ground state can be detected with remarkable sensitivity. The colour centre has been used to study the interaction with electromagnetic radiation with a system with only two or three energy levels. In the current year, the same system has been shown to be invaluable for studying the phenomenon of electromagnetically induced transparency.

In addition to the coherent effects studied in the two principal programs the Group is also involved in numerous spectroscopic studies of solid state systems.

Optical Computing and Processing

The light applied within the dephasing time of an optical transition determines the resultant excited state population, and in the case of an inhomogeneous distribution of transition frequencies, as obtained in a solid, the excited state population will also vary with frequency. For example, if two short light pulses are applied within the dephasing time there will be a sinusoidal variation in the excited state population as a function of frequency. When a single pulse is applied at a time before the excited state decays one obtains the applied pulse plus an echo pulse. With more applied light pulses the distribution of excited state population is more complicated but the subsequent echo is always a restoration of the applied light sequence. In the case of hole burning, a fraction of the excited state population is retained over periods of hours. Thus using hole burning materials, any



pulse sequence can be stored and recalled over the period of some hours. This gives the basis of time domain optical memories and in recent years we have demonstrated that with a phase stable laser the phase as well as amplitude of the applied light can be recovered. In the past year, we have demonstrated the storage and recovery of arbitrary light pulses varying in amplitude and phase. Also with our ability to recover phase information we have shown that it is straightforward to decipher signals previously written in code with an amplitude only system. In a further demonstration, by reversing the order of light pulses we are able to generate time reversal of the stored light signals.

The most significant advance through the year is the development of a new time-domain memory scheme. Previously, to recover arbitrary modulated light pulses it has been necessary to incorporate the sample in an interferometer. However, the interferometer is avoided in the new scheme. The carrier is present all the time. It passes through the sample but does not interact. Modulation of the signal gives rise to sidebands shifted in frequency and these are stored with respect to a short light pulse applied at a small angle. A second equivalent short light pulse recreates the signal on the carrier. This scheme has been patented. *(N.B. Manson and M.J. Sellars)*

Electromagnetically Induced Transparency

The nitrogen-vacancy colour centre in diamond has been used to study electromagnetic induced transparency. This is a phenomenon where application of an electromagnetic field resonant with one transition can cause a complete transparency at the frequency of a second transition and gain can be achieved without population inversion. The practical interests are for effects at optical frequencies. However, the present work, where the fields are at radio frequencies, is more of fundamental interest. The advantage of the current system is that observations are straight-forward and it is possible to introduce further electromagnetic fields and therefore study the perturbation of electromagnetically induced transparency. It is found that the extra field can have no effect, destroy or split the original transparency feature depending on the characteristics of the applied field. In a related study, electromagnetically induced transparency of a dressed state system has been studied. Regular transparency features, derivative features and gain features have been obtained with increasing strength of the coupling field. *(N.B. Manson, E.A. Wilson and C. Wei)*

Spectroscopy

A range of optical spectroscopic studies have been undertaken during the year. These include several continuing projects. With Professor Brian Henderson, Cambridge University, UK and Professor Ann Silversmith, Hamilton College, NY, USA we have studied the spectroscopic properties, upconversion and lasing action of Er doped $KYLiF_5$. With Dr Elmars Krausz and Dr Robin Purchase of the Research School of Chemistry we have studied spectral hole burning of zinc phthalocyanine and with Dr Hans Riesen of the Australian Defence Force Academy we continue to study cobalt doped strontium oxide. The interest in the latter material is as a consequence that the substitutional cobalt ion can occupy one of various sites and the position changed by narrow band optical irradiation. It is considered that this reorientation may provide basis for a memory device.

The spectroscopy of the nitrogen-vacancy centre used for the above electromagnetically induced transparency program has also been studied and the driving force in this case has been to understand why the sensitivity of the latter measurements is so good. The curious feature is the optical pumping causing polarisation of the electronic ground state and we have shown this to be caused by spin selective optical cross over from the triplet to singlet in the excited state followed by fast decay. It is also found that with a specific orientation of an external magnetic field one can obtain polarisation of the nuclear spin states and this leads to the sensitive detection of the nuclear hypefine transitions. *(N.B. Manson, J.P.D. Martin, M.J. Sellars and A. Smith)*

Atom Manipulation

The Atom Manipulation Project has developed a bright (10^{10} atoms/second) beam line source of metastable helium atoms to investigate new atom optical elements to control atomic de Broglie waves. Experiments using the bright beam source to load atoms into hollow optical capillaries have been extended to atom transmission through hollow optical fibres. In the earlier experiments, laser light was coupled into glass capillaries with a uniform refractive index, and was blue-detuned from the metastable helium resonance at 1083 nm to create a repulsive evanescent light field that prevented atoms colliding with the inside fibre wall.

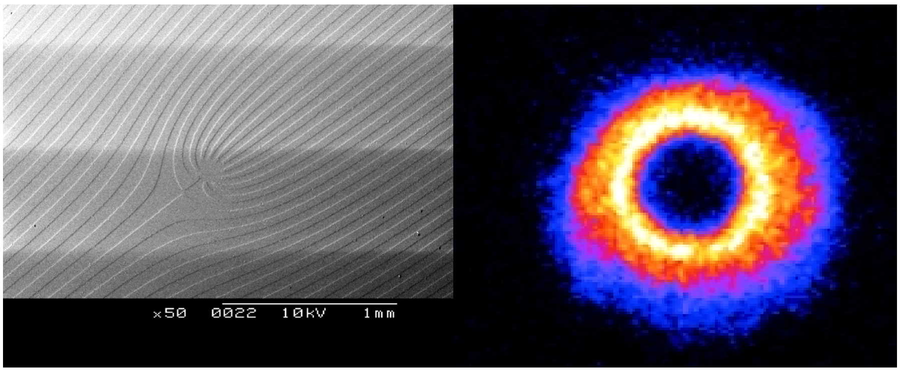
In the latest experiments, hollow optical fibres with a refractive index gradient produced by the Optical Fibre Technology Centre in Sydney were used to confine the guiding laser light in a narrow region around the hole. This enables the selective propagation of the lowest order light modes by varying the laser input coupling conditions. In this manner we have propagated only the lowest order LP01 mode through the fibre, thereby eliminating speckle from multiple-mode transmission and creating a uniform evanescent field around the hole. We have also excited the LP11 mode which upon exiting the fibre propagates as a hollow optical beam, opening up the possibility of an atom funnel into the hollow fibre. Initial experiments have shown evidence for atom transmission through the single light mode fibres and further investigations are continuing.

In order to efficiently couple light into the hollow fibres, we have developed a binary phase mask to create a hollow laser light beam. The charge of the phase mask (between one and ten) can be used to vary the ratio between the width and diameter of the light annulus to optimise the fibre mode matching. Phase mask conversion efficiencies close to the theoretical limit (~40% into each first order beam) were obtained which produced coupling efficiencies into the fibre approaching 70%.

A new metastable helium beam apparatus has been developed as a test rig and for use in atom lithography experiments. This new source was used to extend previous atom lithography experiments to include exposures using metastable neon and argon which were found to be less efficient than metastable helium. It was found that only positive contrast images were obtained using this system, indicating that the new apparatus is subject less to contamination lithography than earlier experiments using the bright metastable helium beam line. *(R. Dall, J. Swansson, N. Sih, D. Tierney, K.G.H. Baldwin; M.D. Hoogerland and S.J. Buckman [AMPL])*

UV Laser Spectroscopy

In parallel with the continuing study of the near-continuum (175 nm) spectrum of the Schumann-Runge band system in diatomic oxygen, this laboratory has commenced a joint project with Macquarie University on the development of new high-resolution laser spectroscopic sources. The goal is to produce a Fourier transform-limited, tunable, solid-state laser based around an injection seeded optical parametric oscillator. This year, we have developed a cw injection seeding system which employs an external cavity diode laser (ECDL) that is tuned by a piezo-electrically controlled grating in the region around 842 nm. The bandwidth of two such ECDLs is measured in a beating experiment to be less than 1 MHz. This is well within the requirement to inject an optical parametric oscillator pumped by a 20-30 ns Nd:YAG pulse possessing a transform limited bandwidth of several 10's of MHz. *(K. Baldwin, M. Kono; B.R. Lewis and S.T. Gibson [AMPL])*



Left: SEM Image of a Charge 10 binary phase mask (2mm wide) and Right: "hollow" laser beam created by diffracting a Gaussian beam from the mask

Staff

Professor and Head of Department

Barry Luther-Davies, BSc PhD S'ton, SIEE, FAIP

Senior Fellows

Neil Manson, MSc PhD Aberd

Wieslaw Krolikowski, MSc PhD Wars (from July)

Fellows

Andrei Rode, MSc PhD Mosc (ARC QEII Fellowship)

Ken Baldwin, MSc, DIC PhD Lond, FAIP

Weislaw Krolikowski, MSc PhD Wars (until July)

John Martin, BSc PhD NSW (until June)

Anna Samoc, MSc PhD Wroc

Marek Samoc, PhD DSc Wroc

Research Fellow

Robbie Charters, BSc Nott, PhD Cranfield (until July) (Australian Photonics CRC)

Postdoctoral Fellows

Anke Freydank, Dipl.-chem. Dr.rer.nat (from January)

Reiner Friedrich, Dipl.-chem. Dr.rer.nat (from April) (Australian Photonics CRC)

Ruth Jarvis, BE BSc (from April) (Australian Photonics CRC)

Max Lederer, BE FH Regensburg, ME UNSW, PhD (ARC Fellowship)

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Changjiang Wei, BSc Hebei MSc Changchun, PhD (until September) (ARC Fellowship)

Congji Zha, BE Jingdezheng, ME WUT, PhD Sydney (from June) (Australian Photonics CRC)

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Graham Atkins, BSc PhD Sydney

Byong Bae, PhD Arizona (until July)

Robbie Charters, BSc Nott, PhD Cranfield (from July)

Darran Edmundson, BSc Waterloo, PhD Simon Fraser (until March)

Yue Gao, BE PhD, Strathclyde

Eugene Gamaly, PhD DSc Mosc (from November)

Dragomir Neshev, MSc, PhD Sofia (from August)

Yanjie Wang, BSc Harbin, PhD

Nassar Zakery, BSc Shiraz, PhD Edinburgh (until October)

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Alex Boiko, PhD, Kiev Polytech

Roger McMurtie, B Appl Phys CCAE, MSc Essex, Grad Dip Comp Studies CCAE (from April)

David Pulford, B.Sc, PhD (from April)

Head Technical Officer

Ian McRae

Senior Technical Officers

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Mike Pennington, AssocDipAppSci&Inst CIT

Anita Smith, BSc Flinders

Technical Officers

John Bottega

Maryla Krolikowska

Therese Martin (Australian Photonics CRC)

Departmental Administrators

Karen Montefiore (until February)

Lesley Elliott (from February until May)

Kristina Milas (from May)

Nuclear Physics

Professor George Dracoulis
- Head of Nuclear Physics

http://wwwrsphysse.anu.edu.au/nuclear

The Department operates the premier laboratory in Australia for accelerator-based research in nuclear physics, providing and developing facilities for national and international outside users, as well as for the staff based in the Department. The facilities are used for postgraduate and postdoctoral training over a wide range of research, from basic to applied.

Research Summary

The imperatives for fundamental studies of the nucleus derive from its properties as a special, quantal, many-body system. While it contains only relatively few particles, it can exhibit both single particle and collective properties from competing motions which are often delicately balanced. The characteristic levels can be at comparable energies and observable as individual quantum states, which in many cases interfere and mix. The study of such properties falls into the province of nuclear spectroscopy whereas the wide range of complex interactions which occur between colliding energetic nuclei is the subject of nuclear reaction dynamics. In these, the varied internal nuclear degrees of freedom couple to the relative motion, hence by both selecting nuclei of different structure and by tailoring the collision conditions, different aspects of the physical processes can be emphasised. Studies of nuclear dynamics therefore have a unique role to play in understanding the interactions between complex objects.

Given these imperatives and the opportunity to apply new accelerator and detection techniques to benefit other areas of science, the research program is continually being developed and currently includes

- Fusion and Fission Dynamics with Heavy Ions
- Nuclear Spectroscopy
- Nuclear Moments and Hyperfine Fields
- Perturbed Angular Correlations and Hyperfine Interactions applied to Materials (PACM)
- Accelerator Mass Spectrometry (AMS)
- Heavy Ion Elastic Recoil Detection Analysis (ERDA)

Success in such a broad range of activities relies heavily on the ability of the 14UD electrostatic accelerator to provide nuclear beams of a range of masses, precisely defined in energy and time. These characteristics result in an efficient and flexible tool for colliding nuclei, and for creating new nuclear species, thus enabling comprehensive studies of both nuclear structure and nuclear dynamics. The accelerator itself, and many of the techniques and instruments developed for basic research are used in high-sensitivity applications. This year has seen consistent activity in all areas using a wide variety of beams. Higher energies for heavier ions are available from the Linac booster which is still being developed to deliver beams to all experimental stations. To improve the performance of the Linac, a program of re-plating of all resonators is currently in progress, with the aim of increasing the high-field limits.

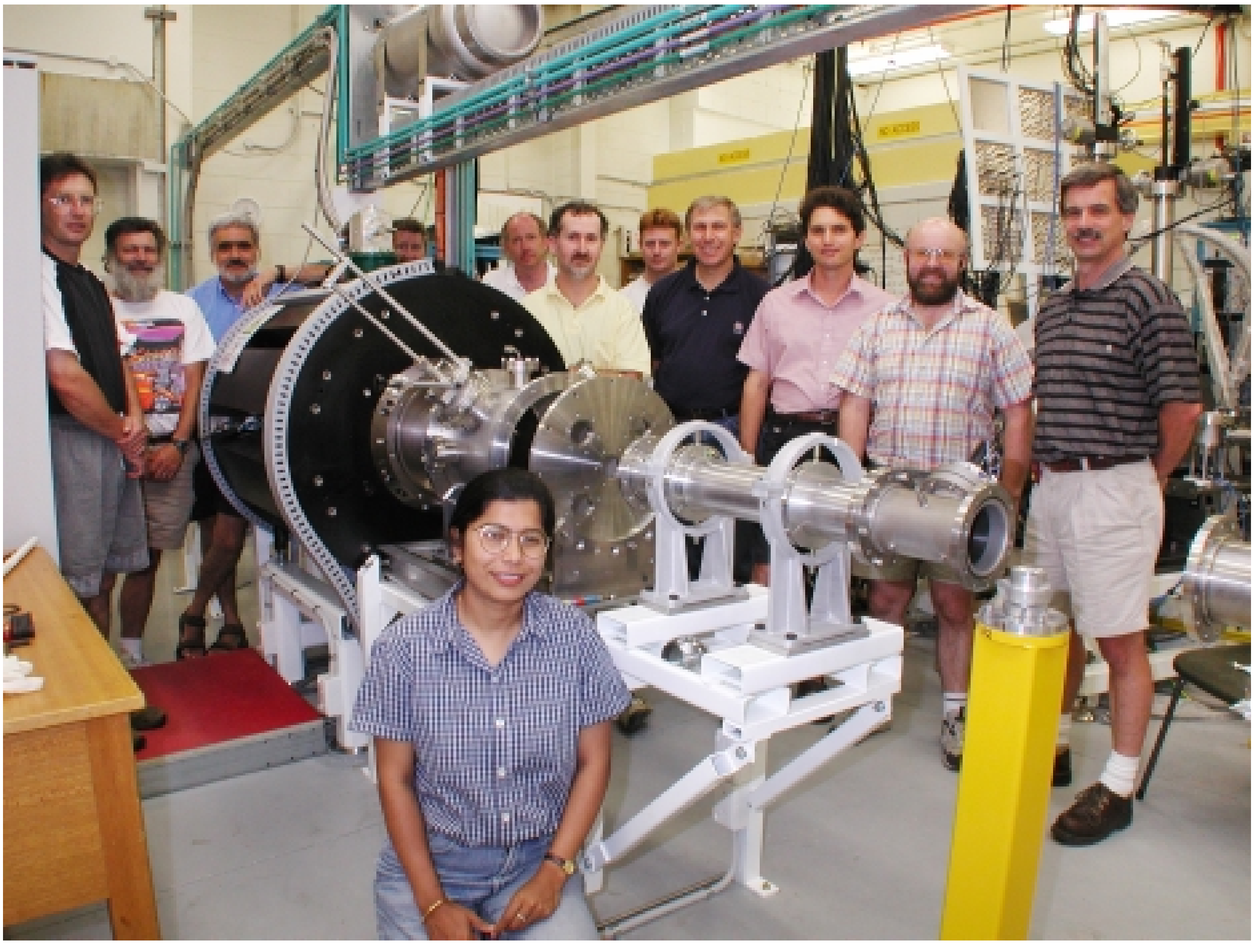
Much of the research is collaborative involving other departments, research schools, universities and institutions. This year, extensive use of the facilities was again made by outside users, including UK scientists who have formal access through the ANU-EPSRC agreement, and US scientists funded through the National Science Foundation. As well as experiments carried out on the local facilities, each of the research groups has active collaborations with outside groups and in a number of cases make use of instrumentation on overseas facilities, complementing the local program.

The need to maintain international competitiveness, at the same time as providing facilities for other users, relies on continuing attention to detector instrumentation and accelerator and ion source technology. Recent enhancements of the research capabilities which affect the accessibility of the facility to outside users include development of a more flexible data acquisition system capable of handling larger multiple-element high-resolution detector arrays and the concomitant high count rates. This is nearing completion, and is in use for some experiments. In the fission-fusion area, the new fusion product separator SOLITAIRE based on a superconducting solenoid, has been installed and tested off-line. Commissioning with heavy beams is planned to occur in early 2001. The majority of funding for both of the above projects was won through earlier bids to the ARC Research Infrastructure, Equipment and Facilities (RIEF) scheme. In the spectroscopy area, augmentation of the g-ray array CAESAR, the central tool of this pursuit, is also in progress with funding support from the University Major Equipment Committee split over two years. Again, completion of this project, which will bring much higher efficiencies, is anticipated for mid to late 2001. The other main area of basic research, Nuclear Moments and Hyperfine Fields, was also successful in obtaining support for new instrumentation through this year's RIEF bid for funding in 2001, the aim being to provide new instrumentation for the study of electric and magnetic fields surrounding atomic nuclei in solids. The Department and specifically the Accelerator Mass Spectrometry group program will also benefit directly from the School's success in its bid to the Institute Planning Committee for long-term funding for new directions in Environmental Studies.

Staff changes in the AMS group included the move of Richard Cresswell to an appointment at the Bureau of Rural Sciences, the arrival of Stephen Tims from Jabiru as a Research Fellow, and of Guaciara dos Santos who is funded as a postdoctoral fellow by the Brazilian Government, and the continuation of a long-term visit by Mariana di Tada from Buenos Aires. Simon Mullins of the Spectroscopy group took up an appointment at the National Accelerator Centre in South Africa and Paul Davidson re-joined the group for a period to work on the Data Acquisition project. Mahananda Dasgupta of the fission/fusion group, who took up an ARC QEII position in 1999, was promoted to Fellow and Heiko Timmers (ERDA) who was an ARC postdoctoral fellow was also promoted, in his case to Research Fellow. Clyde Morton (fission/fusion) won an ARC postdoctoral fellowship this year and was also promoted. The sudden death of Trevor Ophel in the middle of the year was a major blow to the Department and to the ERDA group in which Trevor had been very active. (A short obituary follows this report.)

Staff were housed this year in the refurbished office block. Further restructuring of the Accelerator building to meet the needs of users for detector development and testing and sample preparation etc. has begun and will continue through 2001, with funding from the University's Capital Management Plan.

More details of all aspects of the Departments' activities and research studies, some of which are sketched out below are available in the Department Annual Report for 2000 (ANU-P/1443), available on request, and on the Department web page (http://wwwrsphysse.anu.edu.au/nuclear).



The SOLITARE team, having just installed the 6.5T superconducting solenoid on a Linac beamline

Fusion and Fission Dynamics with Heavy Ions

Studies of the dynamical interactions which couple internal nuclear properties to collective motion, either weakly through a few states, as in fusion, or very strongly, as in the stochastic process of fission.

The activities of the group have been focused on understanding nuclear fusion and fission dynamics, and the dynamical interplay between them. Such effects are a manifestation of the mesoscopic nature of the nucleus, displaying phenomena on the boundary between quantum and classical physics.

A comprehensive study of the fission and other decay modes of the compound nucleus ^{216}Ra has recently been completed. By forming the nucleus using three different fusion reactions, with ^{12}C, ^{19}F and ^{30}Si beams at energies chosen to result in the same excitation energy and angular momenta, it was found that the fission decay properties depend in a systematic way on the mass ratio of the two fusing nuclei. These results lead to the surprising conclusion that even for the ^{19}F + ^{197}Au reaction at low beam energies, a significant fraction of collisions do not lead to an equilibrated compound nucleus.

Neutron transfer is expected to play an important role in the fusion dynamics of very heavy systems. The effects of positive Q-value transfers on fusion have been explored with measurements of quasi-elastic scattering for ^{32,34}S on ^{208}Pb at backward angles. Complementary measurements of sub-barrier fission cross sections have also been carried out and we have been able to show that the barrier distributions extracted from the excitation functions show differences which correlate with the neutron pick-up Q-values.

Following on from our previous work which elucidated the effects of static deformation of the target nuclei on fission anisotropies, a study of the influence of nuclear spin in the entrance channel on fission anisotropies has been initiated, with encouraging results from experiment and calculation. These studies focus on the fission fragment angular anisotropy as a measure of the deviation of the fission axis from the normal to the angular momentum (the unique fission axis for a macroscopic object), which depends on fluctuations in the dynamical trajectories.

Investigation of the influence of break-up channels on fusion has continued. For the fusion of ^{7}Li and ^{6}Li with ^{209}Bi, significant suppression of fusion has been measured at energies above the fusion barriers. This is attributed to breakup of the loosely bound projectiles before reaching the target nuclei. Substantial suppression, which we have also seen in the fusion of ^{9}Be with ^{208}Pb, has not been observed by others in the fusion of ^{9}Be with ^{70}Zn, suggesting that breakup, where observed, may be Coulomb dominated. Because of contradictory results obtained elsewhere for the fusion of ^{6,7}Li with ^{12}C, in which Coulomb effects would be insignificant, we have carried out measurements for these systems. Our results suggest that the discrepancies are probably caused by experimental difficulties in detecting low energy fusion products in the direct detection methods, and hence a loss of efficiency and a likely underestimation of the fusion yield.

Future research will focus on using the new solenoid, SOLITAIRE, for separation of fusion products, once the detection system is complete. The solenoid itself has been installed and successfully commissioned and considerable effort has gone into designing the ancillary apparatus. First tests with beam are planned in early 2001. *(D.J. Hinde, M. Dasgupta, C.R. Morton, H. Timmers, A. Mukherjee, J.O. Newton, A.C. Berriman and R.D. Butt)*

Nuclear Spectroscopy

Focusing on the properties of individual quantum states in nuclei and the identification of new nuclei using g-ray, electron, particle and time-correlated techniques.

The program of spectroscopic studies aimed at deformed nuclei close to stability, in a region where multi-quasiparticle intrinsic states compete with rotational excitations has continued, the main results being assignment of isomers in ^{176}Lu with complex decays. We have been able to show that, for this case at least, the anomalously fast decays are attributable to local mixing, and not to a dilution of the K-quantum number. Other experimental studies in this area during the year have mostly involved collaborative work on identifying and characterising multi-quasiparticle high-K states in rhenium nuclei, to provide more comprehensive information on both decay anomalies and configuration effects on rotation. In a different region where the nuclei are soft and very susceptible to triaxial deformations, the main focus has been the measurement and analysis of cases which might show evidence for predicted chiral (or aplanar) rotation modes.

Our long-standing studies of shape co-existence in the neutron-deficient lead isotopes have also developed with electron measurements to define multipolarities in ^{190}Pb, whose level scheme is dominated by long-lived isomers. Substantiation of the enhanced E3 decays proposed previously has redirected our attention to anomalous rates observed for specific spin-flip proton transitions in both lead and polonium isotopes, which we have now interpreted as new evidence for oblate deformations. More studies in this region are planned for 2001. Further, measurements to identify states above the isomers identified previously in ^{188}Pb and proposed as manifestations of shape co-existence, have been pursued with experiments using Gammasphere at the Lawrence Berkeley National Laboratory.

In the area of instrumentation we are persisting with development of the electron-detector array, HONEY, to be used in the superconducting solenoid for broad-range electron-electron coincidences, particularly of very heavy nuclei. Some progress has been made but further technical improvements are needed to make the system usable in a routine fashion. As indicated earlier, the g-ray array CAESAR is also being augmented with funding obtained in 1999 but spread over two years; considerably improved efficiency should be available during 2001. Parallel developments in the data acquisition system required to cope with the higher rates and to improve generally the flexibility for using ancillary detectors are well advanced. *(G.D. Dracoulis, A.E. Stuchbery, A.D. Byrne, T. Kibédi, R.A. Bark, T.R. McGoram, J.C. Hazel and A.M. Baxter [Physics, The Faculties])*

Magnetic Moments and In-Beam Hyperfine Interactions

The large angular and linear momenta involved in heavy ion reactions is used to facilitate various techniques to study nuclei or to probe atomic environments.

The research program this year has included aspects of condensed matter research, but the main emphasis has been on the measurement and interpretation of nuclear magnetic moments.

A program to study the effective hyperfine fields acting on impurity atoms implanted into gadolinium hosts has commenced in collaboration with solid-state physicists from the Australian Defence Force Academy (ADFA) and the Freie Universität, Berlin. After an initial set of measurements on Tm, Yb, and Ir in Gd near 90 K, it became clear that more extensive studies as a function of temperature would be needed to interpret the data properly. This requires new apparatus. A successful RIEF proposal with collaborators from ADFA, The Faculties and Melbourne University, will allow these studies to continue when new instrumentation comes on-line in 2001.

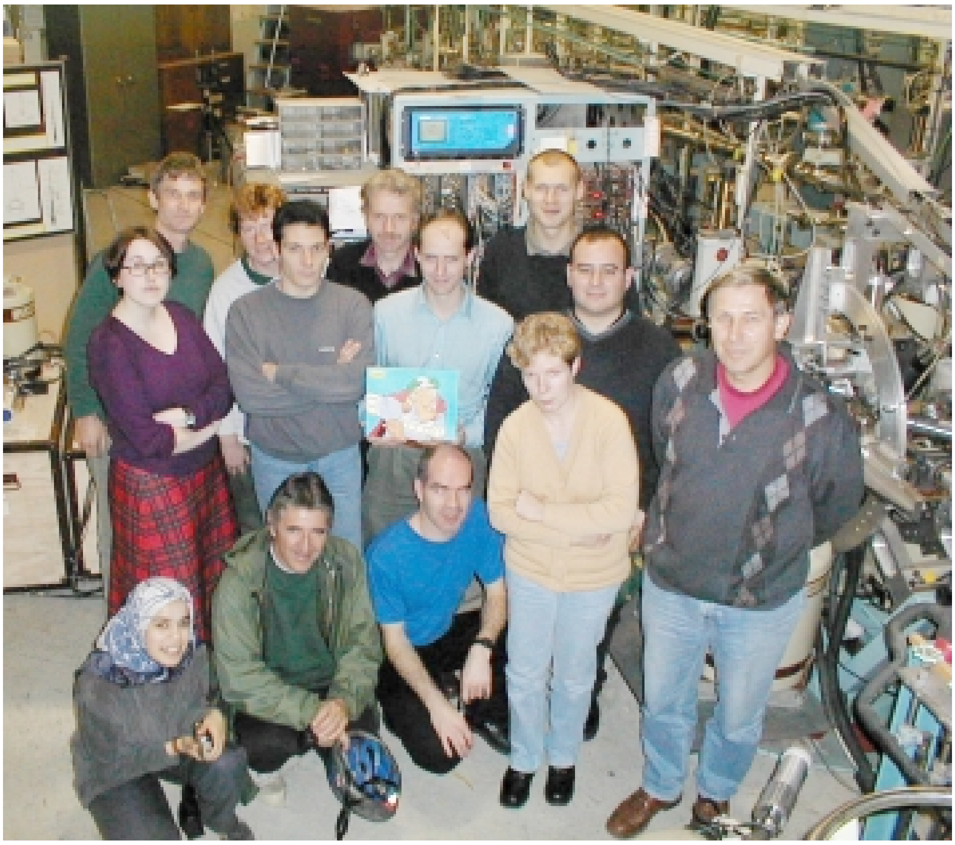
Towards the end of 1999 the first set of measurements using in-beam perturbed directional correlation techniques in the CAESAR array were performed. The analysis of these data, which has required several technical developments, is near completion. An exciting prospect has been discovered in the analysis of the combined effects of a magnetic field and an electric-field gradient experienced by nuclei implanted into gadolinium hosts. Apparently the results are sensitive to both the magnetic dipole moment and the electric quadrupole moment of the nucleus. Measurements of nuclear quadrupole moments may now be possible in a previously unexplored regime.

Experimental studies in collaboration with colleagues from Michigan State University and Rutgers University have examined the magnetic moments of excited states in nuclei near semi-magic nuclei with closed neutron shells. A systematic study of the magnetic moment behaviour in such nuclei in terms of the shell model is underway to examine the effects of the effective nucleon-nucleon interactions and the size of the basis space. The higher-spin states near closed shells have relatively pure configurations and limited basis calculations are adequate, however the lower spin states present a greater challenge to theory because they show considerable collective components even when there are only a few valence nucleons. *(A.E. Stuchbery, A.P. Byrne, G.D. Dracoulis, R.A. Bark and M.P. Robinson)*

Perturbed Angular Correlations and Hyperfine Interactions in Materials

Implantation of long-lived nuclear species with known nuclear moments into special materials probe properties of the materials through the perturbation of the nuclear ensemble by the electric and magnetic fields.

The study of defect configurations in semiconductor materials characterised with the Perturbed Angular Correlation (PAC) method has continued this year with sequences of measurements on Ge substrates varying ion dose, and background dopant type and concentration. In all cases Ge samples were prepared to provide a near constant background dopant concentration of ª1 in $10^{17}/cm^3$ over the region exposed to ^{111}In. The radioisotope was introduced into the sample by a direct production/implantation technique using beams from the 14 UD accelerator. Following annealing, defects were then introduced into the sample using Ge beams from the EME Implanter at energies chosen to reproduce the depth distribution of the ^{111}In.



Visitors to Nuclear Physics with Spectroscopy Group staff during an experiment. left to right: Back Row Phil Walker (Surrey) Alison Bruce (Brighton) Aidan Byrne (Nuclear), Carl Wheldon (Liverpool) Centre Row: Monica Caamano (Surrey) Antonio Emmanouilidis (Brighton) Dave Cullen (Manchester) Nicolas Orce (Brighton) Front Row: Hasna El-Masri (Surrey) George Dracoulis (Head, Nuclear) Zsolt Podolyak (Surrey) Judith Hazel (Nuclear) Tibor Kibedi (Nuclear)

Two well-defined interaction frequencies at 50 and 390 MHz are clearly evident in all measurements, corresponding to two distinct defect configurations. In previous studies these defects have been associated with indium-vacancy or indium-interstitial configurations. In the present studies we have varied the background dopant species and concentration. The results show a surprising independence on the defect fractions observed for the undoped, Ga doped, As doped and In doped samples, in contrast with previous studies which show a strong variation of defect produced as a function of the Fermi level. If such results are correct they call into question the earlier association of these interaction frequencies with particular defects and suggest that the formation of the In-vacancy complex is not the result of elastic interaction between an In acceptor and a neutral vacancy. Work is continuing to characterize these defects and relate the results of our work to recent first-principles calculations of defects in germanium. *(A.P. Byrne; M.C. Ridgway and C.J. Glover [EME])*

Accelerator Mass Spectrometry (AMS)

Uses the combination of a high efficiency (small sample) ion source, tandem acceleration, and heavy-ion detection and identification techniques only possible with relatively high-energy ions, to make highly-sensitive measurements of low abundance isotopes.

Demand for AMS measurements continues to be spread across a broad spectrum of isotopes including ^{10}Be, ^{14}C, ^{26}Al, ^{32}Si, ^{36}Cl, ^{41}Ca, ^{59}Ni, ^{99}Tc, ^{236}U and isotopes of plutonium, with nearly a thousand samples processed this year. There was less emphasis on ^{36}Cl, but this was balanced partially by an increase in the number of measurements of heavy elements, particularly plutonium. First measurements of ^{236}U were also performed in the course of the year in collaboration with the University of Manchester. As in previous years, fields of application were diverse, and ranged across dating of early human occupation of Australia and volcanic eruptions in New Zealand, biomedicine, tracing of releases from nuclear reprocessing plants in Russia and the UK, chronologies for marine and lacustrine cores, meteoritics, and the behaviour of aluminium in soils subject to acid rain.

Collaborative studies have involved a large number of users and contacts including long-term visits by postdoctoral staff funded under a Brazilian Government fellowship, from Argentina, and locally from the Bureau of Rural Sciences. A combined group from Manchester University and Oslo was involved in developing techniques for the measurement of ^{236}U and in the successful application of the techniques to measurement of a depth profile from an estuarine core near Sellafield (UK). A large number of plutonium samples were also measured for various projects related to tracing discharges from various reprocessing plants, and a suite of ^{26}Al samples was measured for a study of aluminium migration from different soil types under the influence of acid rain. Other visits included that of a group from Middlesex University, who brought with them, and assisted with the measurement of, a series of ^{26}Al samples, as well as a suite of ^{244}Pu samples for a major lung uptake study for the National Radiation Protection Board of the UK.

Considerable effort continues to go into ^{10}Be for a project on landscape denudation and sediment storage at a range of scales

Tessica Weijers, a Nuclear Physics/EME PhD student, working in the target area throughout the Australian continent. This project is a collaboration with RSES, and a substantial data set has now been accumulated and interpreted. Measurements to complete a series of depth profiles of ^{10}Be in soils from an undisturbed landscape near Canberra were also carried out during the year.

On the ^{14}C front, the rigorous pretreatment regime developed for charcoal has been tried on ancient wood with good success, permitting the definitive dating of a controversial volcanic ash layer in New Zealand. Work continues as well on ancient human occupation sites in Australia. A chronology for a marine core off the NW coast of Australia, which is an important area for ocean circulation models because water flows through here from the Pacific into the Indian Ocean, has been established for the past 20 ka by dating a single species of foraminifera hand picked from the core. On land, a radiocarbon chronology for a lacustrine/ peat bog core from Lynch's Crater in NE Queensland has been determined back to 48 ka BP. This core preserves an excellent vegetation record of the area throughout the last glacial cycle. In particular, it records an abrupt increase in charcoal concentration at about 40 ka BP, which may be evidence for increasing use of fire by humans at about that time.

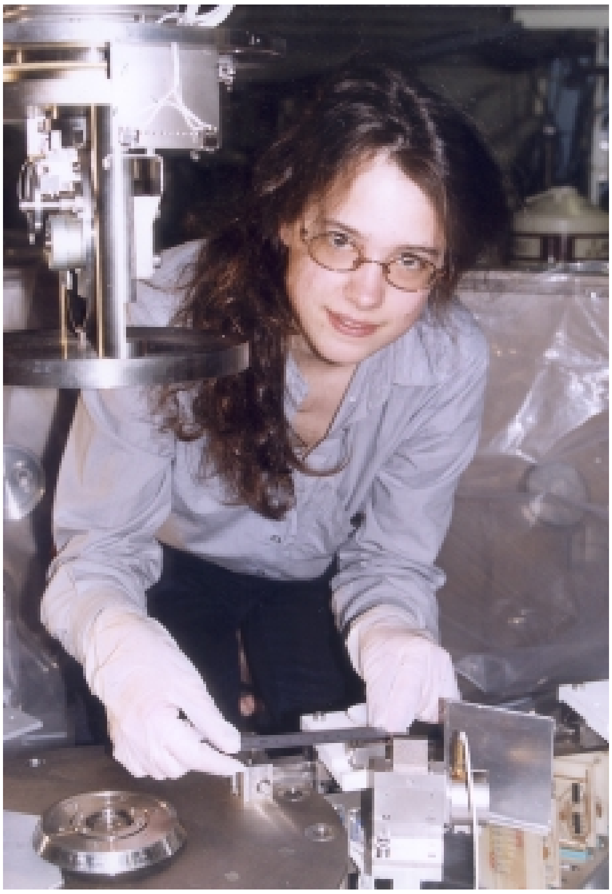
Although proof of principle for ^{41}Ca was demonstrated several years ago, there had been no demand for ^{41}Ca measurements until this year, but interest is now coming from two directions: meteoritics and biomedical. In meteorites, the ratio of ^{41}Ca/^{36}Cl is a useful indicator of time of fall, since it decays with an effective half-life of 380 ka. In biomedicine, the interest is in investigating the effect of various treatments for bone loss by measuring changes in the daily output of ^{41}Ca from people whose skeletons have been labelled with this very long-lived isotope. *(L.K. Fifield, R.G. Creswell, S. Tims, P.A. Hausladen, M.L. di Tada and G.M. dos Santos)*

Heavy Ion Elastic Recoil Detection Analysis (ERDA)

Toward absolute, non-destructive and complete compositional depth-profiling of materials by exploitation of the large scattering cross-sections and stopping powers for high energy heavy ions in solids.

The research activities in this area included materials studies, efforts in technique development and measurements related to ion-material interactions. In addition, aspects of the response of semiconductor detectors have been explored experimentally.

The characterisation of doped silica films for use in integrated optics applications, reported in previous years, has continued. In a collaborative project with the University of New England, compositional analysis was performed for plasma-nitrided austenitic stainless steels. In collaboration with Macquarie University, GaN films were grown on silicon and sapphire by plasma-assisted laser-induced vapour deposition and analysed. In this context the beam-induced desorption of nitrogen, which is a major limitation for ERDA of these materials, is being investigated. Ultra-thin, 1-5 nm, silicon dioxide films are of interest as gate dielectrics in the next generation of microelectronic devices. Measurements of such films were undertaken for comparison with other analytical techniques, including transmission electron microscopy and medium energy ion scattering. Thin silicon nitride and oxynitride layers are also of interest as dielectric layers in modern electronic devices and the oxygen, nitrogen and hydrogen content of such materials was measured as part of two collaborative projects. (Other materials studies work pursued this year are given as part of the Research Summary of the Department of Electronic Materials Engineering.)



Ms Tanja Schuck, a student from Germany, setting up equipment in the 2m scattering chamber, to study the fusion of atomic nuclei

The project on the pulse height deficit of gas ionisation detectors, reported last year, has been extended using a simpler gas ionisation detector. Gas ionisation detectors were originally developed for nuclear physics research but have more recently found use in nuclear techniques of analysis including heavy ion ERDA. This is largely due to their excellent energy resolution and their insensitivity to radiation damage. However, it is known that the response of gas ionisation detectors is not independent of ion species. For a given ion energy the pulse amplitude decreases with increasing atomic number Z, leading to a so-called, pulse-height deficit. To investigate and isolate the causes of this effect, the range of ions and energies studied has been greatly extended and the expected contributions of energy loss in the window and energy missed due to non-ionising collisions, examined in detail and corrected for.

Accurate energy loss and straggling data are required for quantitative ion beam analysis. Unfortunately, the accuracy of such data for high-energy heavy ions is limited to ~20%, imposing limits on techniques such as heavy ion elastic recoil analysis and heavy-ion backscattering spectrometry. In a collaborative study with the University of Lund and the University of Newcastle, measurements of the stopping power and energy straggling of a variety of heavy ions in Si have been undertaken over the energy range 1 - 2 MeV/amu.

Studies are also being carried out on the response of Silicon detectors themselves. They currently play an important role in heavy ion detection including applications such as ERDA, but the response of these detectors is also known to depend on the ion mass. A deeper understanding of the interaction of heavy ions with silicon detectors is required to understand this effect. Measurements were undertaken using the 14 UD accelerator to extend previous results to heavier ions and higher energies. These measurements showed a complex dependence of the energy required to create a detectable electron-hole pair, on the ion mass. In particular, it was found that this energy first decreased and then increased with increasing ion mass, so that a pulse height surplus was recorded for masses up to 80 amu while there was a pulse height deficit for higher masses. This has important implications for precision measurements using surface barrier detectors and further studies of the underlying mechanisms are in progress. *(H. Timmers, T.R. Ophel, T.D.M. Weijers and R.G. Elliman [EME])*

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David Hinde, BSc Manc, PhD, FAIP

Andrew Stuchbery, BSc PhD Melb, FAIP

Reader

Aidan Byrne, MSc Auck, PhD, FAIP

(joint appointment with Department of Physics, The Faculties)

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Tibor Kibédi, PhD Debrecen

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Clyde Morton, BSc Sydney, PhD (from June) (ARC Fellowship)

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Anjali Mukherjee, MSc, PhD Calcutta

Heiko Timmers, Dipl. Phys. Munich, PhD (until July) (ARC Fellowship)(jointly with Electronic Materials and Engineering, and the Department of Physics and Theoretical Physics, The Faculties)

Visiting Fellows

Ragnar Bengtsson, University of Lund, Sweden (January-February)

Peter Butler, University of Liverpool, UK (January-February)

Richard Cresswell, Bureau of Rural Sciences

Mariana di Tada, MSc, PhD Buenos Aires

Guaciara dos Santos, CNPq, Universidade Federal Fluminense, Brazil

Tobias Funk, Free University, Berlin, Germany (January-February)

Simon Mullins, BSc Leicester, D.Phil York (January)

John Newton, MA PhD Camb., DSc Manc., FAA (Emeritus Professor)

Trevor Ophel†, BSc Adel, PhD (Emeritus Professor) (until June)

Ray Spear, PhD DSc Melb, FAPS, FAIP (Emeritus Professor)

Ross Taylor, MSc NZ, PhD Indiana, MA DSc Oxf FAA Hon. FGS, Hon. FRSNZ (Emeritus Professor)

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Research Officer

Gordon Foote, BSc Lond, PhD

Research Assistant

Paul Davidson, BSc, MSc Auckland, PhD (from May)

Engineer

Nikolai Lobanov, BSc Moscow, PhD St Petersburg

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Alan Harding

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John Kennedy

Lorenzo Lariosa

Alistair Muirhead

Andy Rawlinson

Bob Turkentine

Howard Wallace

Departmental Administrator

Marj O'Neill

† = Deceased

Trevor Ophel 7.9.1934 – 17.6.2000

The nuclear physics community lost one of its stalwarts with the sudden death of Trevor Ophel, at his Broulee property on June 17th. Trevor was born in Adelaide on September 7th, 1934 and at the time of his death, was actively pursuing research as Emeritus Professor at the Australian National University and Visiting Fellow in the Department of Nuclear Physics. When he officially retired at the end of 1999, he was the longest serving member of the Research School of Physical Sciences and Engineering at the ANU.

Trevor started his career in physics at an early age with an honours degree in Science from the University of Adelaide and a stint at the "Radio School" in Ballarat during his National Service in the Air Force. He first joined the ANU as a postgraduate student in the fledgeling Nuclear Physics Department in 1955. His thesis on "Scintillation Counter Studies of Photoproton Reactions", was completed in 1958 (at age 23) and conferred in May the following year, making him one of the first few PhD graduates from the Research School of Physical Sciences in the Institute of Advanced Studies. After a period as a Research Fellow at the Cyclotron Laboratory in Harvard he was recruited in 1959 by the Head of Nuclear Physics, Professor (later Sir) Ernest Titterton, to play what came to be a central role in the development of front-line research facilities at the ANU. In Ernie's words, Trevor was to be the "Resident Physicist with the Tandem Generator" reflecting his central role in developing and maintaining front-line accelerator facilities and instrumentation for basic research, a role he continued to play throughout his career. From his earliest contacts he developed a profound understanding of detectors and accelerators of all varieties and it was this background that allowed him to contribute continually to innovations in experimental research, basic and applied, such as the Accelerator Mass Spectrometry (AMS) program at the ANU which he helped to initiate, and most recently the development of the elemental analysis program based on Heavy Ion Elastic Recoil Detection (ERDA). Both have flourished because of Trevor's intimate knowledge of detectors and accelerators.

In his earlier career, Trevor built an international reputation in nuclear spectroscopy, heavy ion reactions, accelerator physics and instrumentation, publishing over 120 papers in the learned journals. He rose through the ranks to become Professorial Fellow in 1982 and while he served for lengthy periods as Acting/Deputy Head, he was formally Head of the Department between July 1988 and July 1992, as well as being acting Director of the Research School on numerous occasions. He took great pride in the emergence of the Heavy Ion Accelerator Facility as a recognised and competitive international laboratory and he took particular pride in its training of PhD graduates over nearly five decades.

In the wider scientific community he served in various capacities, particularly with the Australian Institute of Nuclear Science and Engineering (AINSE) acting on its specialist groups, its council, and as its President from 1997 to 1999. Trevor was a regular participant in the AINSE Nuclear and Particle Physics Conferences and he worked closely with a number of overseas physicists, through visits to the USA and as a host to visitors at the ANU. He was a keen historian and a natural archivist, never throwing anything out. He was a natural choice on the occasion of the ANU's 50th anniversary, to write a history of the Research

Trevor Ophel in his student days (right), pictured here with Ernest Titterton (early 1958)

School of Physical Sciences which he did together with John Jenkin of Latrobe University, also an ex-graduate now turned historian. The result, "Fire in the Belly", published in 1996, was a celebration of one of the Foundation Schools of the ANU and was dedicated to its founder, Sir Mark Oliphant. Trevor followed in 1998 with a history of the Department of Nuclear Physics itself, entitled "A Tower of Strength" which he dedicated to the memory of Ernie Titterton. Both dedications mention the drive, energy and enthusiasm of these pioneers of Science in Australia, qualities which Trevor admired and which he possessed himself, in abundance. Both books provide a unique and pictorial record of the successes and trials of particular areas of scientific research in Australia, particularly nuclear physics.

However, while he overlapped with the pioneers, he was neither one of the old school, nor one of the new guard. Overseas physicists with whom he worked as a regular visitor to laboratories in the USA and whom he hosted in their visits to the ANU probably saw him as the archetypal Australian – weather-beaten, wiry, and pragmatic – crouched on his haunches smoking a cigarette and wearing the ubiquitous sandals. Sandals whatever the season, whichever the continent!

Trevor would not have regretted the suddenness of his passing but he would have appreciated the loss to the field of such a profound "corporate" memory, something which is much undervalued in modern science. That loss has already been keenly felt in the nuclear physics community.

He is survived by his wife of 42 years, Joan, children Margaret, John, Cathy, Susan and Greg, and nine grandchildren.

George Dracoulis 30 July 2000

Optical Sciences Centre

Professor Allan Snyder - Head of Optical Sciences

The Optical Sciences Centre continues to cross boundaries and venture into exciting new domains. Once again, we have received awards and honours, significant publicity and have delivered keynote addresses worldwide.

Research Summary

This year marked a turning point in the Optical Sciences Centre (OSC). We have embarked on a new venture in theoretical brain physics. The intent is to research global aspects of brain processing. The OSC won an institute wide Performance and Planning Fund Grant to amplify our efforts in biological physics and soliton physics. This also complements our new joint Research School of Biological Sciences/Research School of Physical Sciences and Engineering post-doctoral position in the Mind Sciences for research using transcranial magnetic stimulation to induce non-conscious processing.

Achievements of staff include the discovery of exploding solitons; the elucidation of processes in systems far from equilibrium with application to phase transitions, lasers and biological systems; and further exploration in the area of light guiding light technology. The Centre's work on photonic crystals featured in a special issue of *Optics and Photonics News* and was also the cover story of the August issue of *The Physicist*.

The OSC continues to work on linear waveguides and fibre-based optical devices. A novel method for attaching buried channel waveguides to optical fibres is also being developed.

Professor Allan Snyder has been invited to give the Royal Society's Clifford Patterson Lecture in 2001. He has also been nominated as a tall poppy, one of thirteen outstanding Australian scientists of the century, in the Australian Institute of Political Science's Tall Poppy Campaign.

Below we mention only some of our recent activities and collaborations.

Photonic Crystals and Photonic Crystal Waveguides

A new area of research started this year is the study of nonlinear properties of photonic crystals and photonic crystal waveguides, and our first paper in this field has already featured in the special issue of *Optics and Photonics News*. Other results from the group on photonic crystals include a systematic analysis of the existence and stability of nonlinear guided waves, the first theory of optical phase-matching in 2D photonic crystals with quadratic nonlinearity (in collaboration with Professor Solomon Saltiel), and a new method of an efficient harmonic generation in nonlinear photonic crystals (in collaboration with Professor Solomon Saltiel and Dr Martijn de Sterke [University of Sydney]). A general overview of the field of photonic crystals, together with a summary of our recent results on nonlinear photonic crystals, was the August cover story of *The Physicist* (by Professor Yuri Kivshar and Dr Serge Mingaleev). *(A. Sukhorukov and Y. Kivshar)*

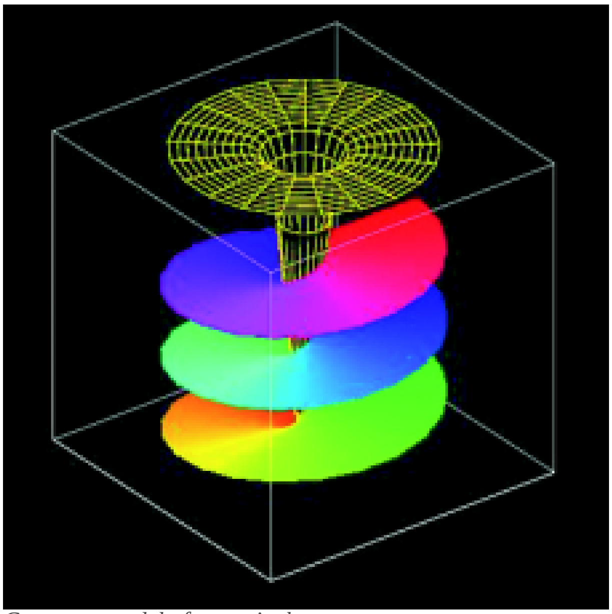
Spatial Solitons and their Interaction

One of the most important research highlights of 2000 is the prediction of a new object in the nonlinear physics, a dipole-mode vector soliton. This is a composite optical beam that carries a dipole momentum and can be understood either as a Hermite-Gaussian guided mode trapped by a soliton-induced waveguide or as a bound state of two simpler solitary waves in a bulk medium, the so-called "molecule of light". This and other more complicated and intriguing objects including quadrupole vector solitons and "necklace" beams have been predicted and demonstrated experimentally (in collaboration with a team from the Laser Physics Centre). This topic has attracted great interest from other groups, with almost simultaneous experimental verifications done at Princeton (USA) and Technion (Israel).

http://wwwrsphysse.anu.edu.au/osc

Optical Vortices

The study of optical vortices is a continuing research activity of our team. This year, several projects have been completed, such as the prediction and analysis of parametric vortex solitons in a medium with quadratic and cubic nonlinearities (such vortices have been recently demonstrated experimentally by Professor P. Di Trapani's group from Italy). Together with our colleagues from the Laser Physics Centre, we have predicted and demonstrated experimentally a new effect in the physics of vortices: the so-called nonlinear Aharonov-Bohm scattering. This result appeared in the special issue of *Optics in 2000* that presents summaries of the most important recent research in optics. *(Y. Kivshar and E.A. Ostrovskaya)*



Computer model of an optical vortex

Dynamics of Bose-Einstein Condensates

Last year the group entered the field of Bose-Einstein condensation (BEC). In November 1999, we organised an international workshop on this topic and hosted several visitors from Spain, New Zealand and Australia. Our first projects in this field were based on the idea of nonlinear modes of the BEC in a trap, first applied to the simplest case of a parabolic trap, but then developed for the case of the Josephson-like oscillations in a trap with two local minima. Tristram Alexander is applying some of the ideas of parametric optical interactions to the theory of atomic-molecular condensates. BEC and atom lasers are the research topics of a new PhD student, Nick Robins, who is also working on the theory of atom lasers with Dr Craig Savage (The Faculties). Honours student, Ben Cusack, has successfully completed a project on the dynamics and stability of the atomic-molecular BEC. *(B. Cusack, T. Alexander, E.A. Ostrovskaya, Y. Kivshar and N.P. Robins)*

Theory of Spatial Optical Solitons

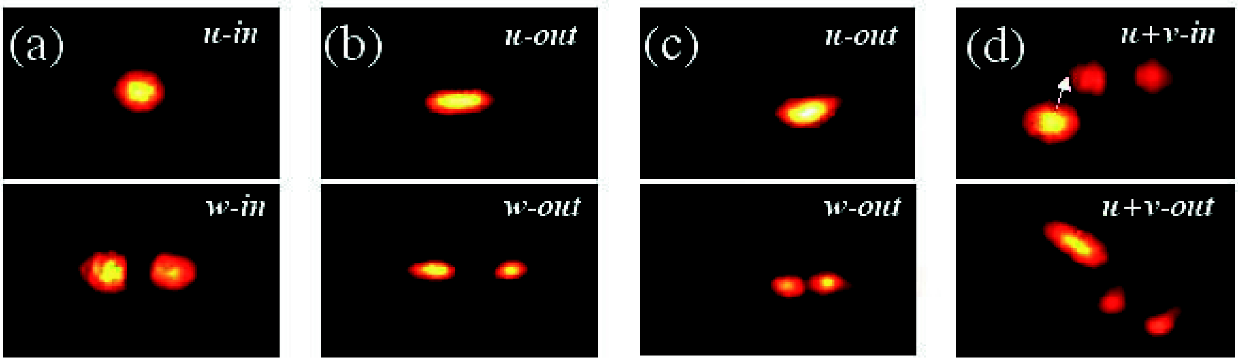
Advances in the theory of spatial optical solitons include a rigorous stability analysis of multi-parameter solitary waves (Dr Dimitry Pelinovsky and Professor Yuri Kivshar), a comprehensive overview of the transverse and modulational instabilities of solitary waves (Professor Yuri Kivshar and Dr Dimitry Pelinovsky), the study of both linear and nonlinear properties of vortex-induced waveguides (Dr Elena Ostrovskaya *et al*), and the first systematic analysis of the stability of nonlinear localised modes and waveguide modes in nonlinear periodic media (Mr Andrey Sukhorukov *et al.*). *(E.A. Ostrovskaya, A. Sukhorukov and Y. Kivshar)*

Systems Far from Equilibrium

The OSC group made remarkable progress in understanding novel processes in systems far from equilibrium. The main feature of these systems is that they include energy exchange with external sources. These cover a variety of phenomena in nature such as convection instabilities, phase transitions, processes in lasers, all-optical transmission lines and even describe biological systems using relatively simple mathematics. Namely, the group reported a discovery of pulsations in localised structures which might take a form of simple periodic pulsations, complicated chaotic pulsations, explosions and slow pulsating translations in space (creeping). The results were published in *Physical Review Letters*. *(N. Akhmediev and A. Ankiewicz)*

Fibres and Fibre-based Optical Devices

A wide range of devices for manipulating and processing light has been investigated, including tapered optical fibres for scanning near-field optical microscopy application, multimode fibres with special refractive index profiles for optimising biosensing applications and photosensitive fibre designs for application to wavelength add/drop devices for dense wavelength division mulitiplexing applications. *(J.D. Love and S.J. Ashby; P. Moar, B. Gibson and J. Katsifolis [La Trobe University])*



Experimental results demonstrating (a,b) the formation of a dipole-mode soliton, and (c,d) its collision with a scalar soliton and the linear to angular momentum transfer

Members of the nonlinear physics group, D. Neshev, N. Robins, E. Ostrovskaya, A. Sukhorukov, T. Alexander and A. Desyatnikov

Waveguides and Waveguide-based Optical Devices

Planar waveguide devices have been designed and analysed covering a range of applications: (i) hybrid polymer-silica devices for maximal thermo-optic response in switching applications; (ii) longitudinal gratings for minimising loss in bent waveguides; (iii) a novel type of reflection grating design to minimise coupling to higher-order modes, and (iv) a two-wavelength add/drop filter using a blazed grating-assisted six-port planar coupler. *(J.D. Love, A. Ankiewicz, S. Tomljenovic-Hanic, R.A. Jarvis and K.W. Gaff)*

Novel Silica-based Materials for Planar Optical Devices

In collaboration with the Space and Plasma Processing Group, a range of new doped silica-based materials have been developed in thin-film form using the HARE PECVD reactor, having a large photorefractive response to exposure to intense UV light. This range includes germanosilicates and stannosilicates, both of which also have a particularly low hydrogen content corresponding to a large reduction in OH absorption at 1400 nm. These materials are therefore highly suitable for the fabrication of planar waveguide processing devices that exhibit low loss over the whole available spectrum for optical communications. *(J.D. Love, K.W. Gaff, R.A. Jarvis and R.W. Boswell [PRL])*

Fibre-to-Waveguide Pigtailing

A novel method for attaching buried channel waveguides to optical fibres is being developed which automatically guarantees minimum splicing loss by suitably etching the fibre and waveguide endfaces to form a peg-in-hole arrangement. This arrangement also ensures the automatic alignment of the cores of the fibre and waveguide irrespective of their alignment relative to the fibre and waveguide cross-section, respectively. *(J.D. Love, S. Law [Sydney University], S.T. Huntington [Melbourne University] and D. Thorncraft [Redfern Photonics Pty Ltd])*

Numerical and Analytical Techniques

Sophisticated commercial software enables the accurate modelling and design of either single devices or a chain of devices, as a service to groups in the School and across the ANU and within the Australian Photonics Cooperative Research Centre. A new technique based on conformal mappings has been developed for the analysis of waveguides and devices that incorporate bends in their designs. *(J.D. Love, A. Ankiewicz, M. Austin [RMIT University] and A.E. Ash [Ericsson Australia Pty Ltd])*

New Initiatives

Brain Physics

The Centre embarked on a new venture, with an international search for a theoretical brain physicist who will research global aspects of brain processing. In addition, a joint Postdoctoral position was offered between the OSC, Centre for the Mind and the Research School of Biological Sciences for research using transverse magnetic stimulation to switch off conscious thought. This research explores and extends the theoretical work by Professor Allan Snyder and Professor John Mitchell which was published in the Proceedings of the Royal Society of London.

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Yuri Kivshar, PhD USSR Acad Sci
John Love, MA Camb, MA DPhil DSc Oxf
John Mitchell, BSc Syd, PhD NSW

Fellow
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Postdoctoral Fellow
Elena Ostrovskaya, MSc Mosc, PhD

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Abbey Hughes (Professor)
Serge Mingaleev
Dragomir Neshev, Sophia U., Bulgaria (from September)
José Soto-Crespo, Instituto de Optica, Madrid, Spain (from December)
Weiping Zhang, Physics, The Faculties (July-September)

Departmental Visitors
Alan Bishop
Akira Hasegawa (Professor)
Todd Kapitula
Alex Nepomnyashchy (Professor)
Dimitry Pelinovsky
Nikolai Rosanov (Professor)
Solomon Saltiel (Professor)

Professional Staff
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Plasma Research Laboratory

Professor Jeffrey Harris - Head of Plasma Research Laboratory

The Plasma Research Laboratory investigates the physics of the fourth state of matter, a subject of fundamental significance as well as of immense practical benefit to humankind.

Research Summary

The Plasma Research Laboratory (PRL) as a Department comprises two groups: the Toroidal Group and the Space Plasma and Plasma Processing Group (SP^3). Its research also directly involves the Plasma Theory Group, through affiliations with the Department of Theoretical Physics, and the Department of Computer Science, Faculty of Engineering and Information Technology. Professor Jeffrey Harris is Head of the Laboratory and the Toroidal Group, Professor Roderick Boswell leads the SP^3 Group, and Professor Robert Dewar leads the Plasma Theory Group.

The Laboratory conducts both fundamental and applied research into the properties of ionised gases (plasmas) constrained by magnetic fields in a variety of geometries, and interacting with electromagnetic radiation over a wide range of frequencies. A feature of the Laboratory is its links between the experimental and theory groups. Its facilities for the study of high- and low-temperature plasmas combined with an integrated theoretical program make it a national resource, and place it among the leading university-based plasma physics laboratories in the world. The Laboratory also attracts a large number of students and collaborative researchers from Australia and overseas.

The Laboratory works in several areas of plasma physics, the longest established of these being in fusion energy and plasma processing of materials. It has pioneered the development of the heliac concept, for containing hot plasma in an externally produced helical magnetic field and built a large experimental realisation of this concept, the H-1NF heliac, which became a Major National Research Facility in 1997. Experiments on this flexible device have already produced results that provide insight into the underlying physics of particle and energy confinement present in both H-1NF and larger, less accessible experimental plasmas.

The second major thrust of PRL is in applications of plasma processing such as the production of computer chips and planar optical waveguides. PRL has developed and patented a novel plasma processing system, known as the Helicon Reactor, which has now been adopted by university laboratories and the plasma processing industry around the world. The Laboratory has made important contributions to the understanding of the basic physics of the helicon-wave source by the careful comparison of experimental results with computer simulation of the nonlinear interaction of helicon waves with plasmas.

Plasma science is by nature multi-disciplinary, and plasma researchers are always on the lookout for new and interesting things to do. The Modulated Solid-State (MOSS) spectrometer developed for the H-1NF by PRL staff and commercialised by Australian Scientific Instruments Pty Ltd has now been installed in overseas laboratories. A provisional patent has been granted for a newly built spectrometer extending the MOSS concept, and a demonstration plasma antenna system developed by PRL in collaboration with the Australian Defence Science and Technology Organization has been constructed. Development of the plasma antenna concept for microwave applications is underway.

The need to visualise the complex geometry of plasma confinement in three-dimensions led Professor Rodrick Boswell and Dr Henry Gardner to conceive of the WEDGE, a two-wall virtual reality theatre that uses simplicity in design coupled with personal computer technology to achieve stereoscopic data visualisation at a fraction of the cost of existing commercial systems. This has resulted in a number of these systems being installed, at the Powerhouse Museum in Sydney, the CSIRO Discovery Centre, and the Australian Defence Forces Academy, Canberra. These developments and others are described in more detail on the PRL web site.

http://wwwrsphysse.anu.edu.au/prl

Development of the H-1 National Facility

Following the completion of the main upgrades to the H-1 National Facility, the H-1NF was operated for 103 days over 29 weeks, recording data for 4,600 shots this year. Of this, approximately 100 shots over 67 days of operation were plasma physics shots, the balance being power supply and machine test shots. The new high-precision 12 Megawatt magnet dual power supply was successfully tested into a dummy load to full voltage (900 Volts) and full current (14,000 Amps) individually. The power supply will ultimately increase the magnetic field of the H-1NF device from its original operating value of 0.2 T to its design value of 1 T. An interactive but secure control interface was implemented to allow operators to exploit the great flexibility of the programmable power supplies. Tests have demonstrated programmable constant or ramping current into H-1NF up to 8,500 A, with variations of a small fraction of one Ampére. This ensures highly accurate magnetic geometry, avoids interference with measurement systems, and minimises induction of current into this inherently current-free plasma configuration. Reliability of the motor-generator, an alternative low power source for the magnet system, was also enhanced this year by installation of new switchgear and controls.

A secondary supply powers the control windings and allows the plasma shape to be varied, under computer control, over a much wider range than possible in conventional stellarators or tokamaks, with the option of varying the current during a plasma pulse. The connections between these supplies and the five windings of the heliac are made in a very flexible and convenient manner through a “patch panel”. This system is capable of carrying 14,000 A for two seconds, and crucial configuration information including total winding inductance, mutual inductance and resistance is passed on to the power supply controller via computer. This enables full exploitation of the wide range of magnetic characteristics accessible to the H-1NF.

This ambitious and unique project, combining a power plant similar to that powering a Very Fast Train (VFT), with the precision and flexibility of a laboratory instrument, was a product of collaboration between H-1NF staff and a number of Australian and international companies. These include: Walsh & Associates, Consulting Engineers, Sydney; ABB-Melbourne; Technocon AG, Switzerland; TMC Ltd of Melbourne (transformer); CEGELEC of Sydney (AC-DC converter); A-Force Switchboards, Sydney (14 kA patch panel) and HOLEC Engineering of Sydney (switchgear).

Plasma operation with magnetic fields up to 0.5 Tesla was achieved this year, enabling the first phase of high temperature plasma operation in which the plasma is heated at the second harmonic of the electron cyclotron resonance frequency. The best results were with RF heating near the ion cyclotron frequency (7 MHz) in Hydrogen and a Hydrogen-Helium mixture. Work on the 28 GHz, 200 kW electron cyclotron heating system continued, as part of the collaboration with Kyoto University and the Japanese National Institute for Fusion Science (NIFS), with testing and enhancing the power electronics, installation of the waveguide and launching systems, and the associated vacuum window. Work on the ion cyclotron range heating system included installation of DC isolation components, and cabling with high power coaxial cable to the launching port. The electron heating system is now ready for first high-temperature plasma experiments.

A number of the sixteen additional vacuum ports have been put to use, some for facility collaborators and others for enhanced diagnostic systems. Development this year included the plasma density tomography system, the optical vector tomography system, the electron cyclotron heating system and the gas injection systems. Experiments for facility users can now be quickly connected, without vacuum interruption, via the newly installed gate valves if required. The cryo-pump, which allows rapid pump-down after a vacuum break, was remounted and commissioned late in 2000.

As a result of infrastructure upgrades, the Facility now has a degree of redundancy in power, heating and vacuum systems. This has allowed a higher level of availability this year. The remaining upgrades to the heating and launching systems, and bringing the machine up to full magnetic field, namely 1 T, will result in only minor interruptions to operation over the next two years.

A number of new plasma measurement systems have been installed or commissioned. A Modulated Optical Solid State (MOSS) camera has been operating routinely since early 2000 and has produced a wealth of new information pertaining to the H-1 plasma dynamics. The tomographic MOSS (ToMOSS) spectroscopy system is now fully installed and was commissioned in September 2000. A new multi-channel spectroscopy system for measurement of electron temperature and plasma fluctuations is also operational while a general survey spectrometer completes the spectroscopic diagnostic suite.

The far-infrared (FIR) scanning interferometer has also been extensively upgraded this year. The 2 mm sweep-frequency interferometer (a standard diagnostic) has been relocated to allow toroidal cross-correlation with the FIR system measurements. A ruby-laser-based Thomson scattering system for electron temperature measurements is also nearing completion. These, and other developments, are reported more fully below.

Toroidal Plasma Physics

Transport and Turbulence Studies in H-1 NF

The physics of particle and energy transport across confining magnetic fields in toroidal plasmas remains one of the hottest topics in plasma physics. Instabilities and turbulence contribute to the particle and energy loss across the magnetic field in the H-1 heliac, as well as in other toroidal plasmas. Sheared plasma flows are thought to modify the turbulence, though the details of this modification at the microscopic level are not yet fully understood.

Experimental studies into plasma transport in H-1 have been expanded in 2000 in several directions: development of new diagnostics for transport and turbulence studies, application of novel signal analysis techniques, and comparative analysis of turbulent transport in stellarators and tokamaks.

Novel probe techniques have been developed to attack several fundamental physics issues related to plasma turbulence. Such as the role of the fluctuations in ion temperature on the plasma thermal conductivity. This problem is closely related to the more general problem of decoupling of the ion and electron thermal transport in plasma confinement experiments. Results obtained in 2000 indicate that the relative level of ion temperature fluctuations may significantly contribute to ion thermal transport. Another work in progress is aimed at experimental evaluation of the degree of the ambipolarity of fluctuation-driven particle transport.

Applications of novel signal analysis techniques to study the dynamics of confinement bifurcations and the associated turbulence modification has been investigated in collaboration with scientists from Central Queensland University. A spectral Fourier-transform-based representation of the turbulent particle fluxes has been reformulated using the wavelet analysis technique. (This helped study the dynamics of the modification of fluctuation-produced fluxes with improved temporal resolution especially important during the confinement transitions in H1-NF)

Finally, a comparative analysis of turbulent transport in different toroidal confinement experiments is being carried out. Comparison of turbulent transport in the H-1 heliac, CHS torsatron (Toki, Japan) and the DIII-D tokamak (San Diego, USA) is in progress and has already produced interesting results suggesting universality of some turbulent transport effects previously observed in H-1. *(M.G. Shats, W. Solomon, H. Punzmann)*
http://rsphysse.anu.edu.au/~mgs112/html/transport.htm

Remote Data Access

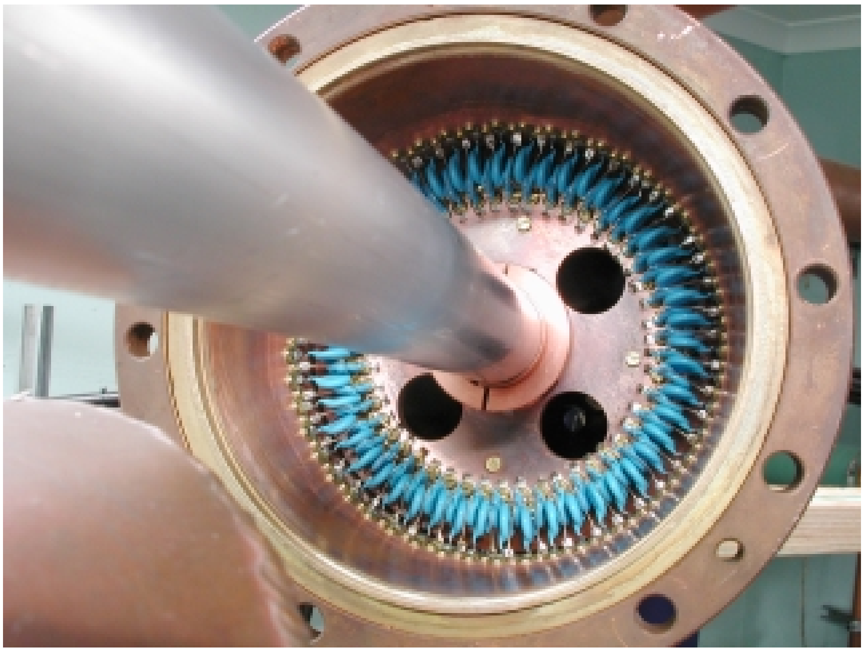
Java-based remote viewers for data produced by the H-1NF magnetic field and power supply were developed in 2000. These transfer some of the processing load from the H-1NF server computer to a client's personal computer. Work also continues on a more comprehensive Java viewer incorporating elements from a similar project at the University of Padua, Italy. Remote access, using "Virtual Network Computer" (VNC) remote "virtual desktop" software, is very useful for collaborators and the Facility's users at remote sites. The ability for shared use of a common desktop, graphical displays and mouse is valuable when collaborators are not in the same location. *(B.D. Blackwell and D. Price)*

H-1NF Data System

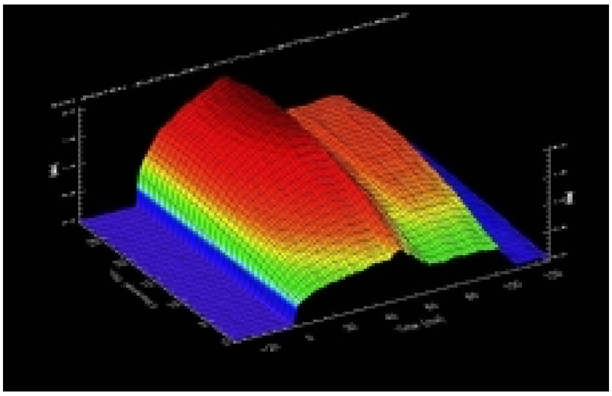
The MDSPlus data system, jointly developed by several international plasma fusion laboratories, was implemented in 1999 as the main H-1NF database during a visit by Thomas Fredian from the Plasma Fusion Centre at the Massachusetts Institute of Technology in the US. MDSPlus is a powerful self-describing hierarchical database particularly suited to time series data. The system, used in many large laboratories, runs under OVMS, UNIX and on personal computers, has transparent loss-less data compression, and a convenient graphical interface. More than ten gigabytes of data in 7,000 pulses have been taken since installation. *(B.D. Blackwell and J. Howard)*

Magnetic Design and Optimisation/Advanced Stellarators

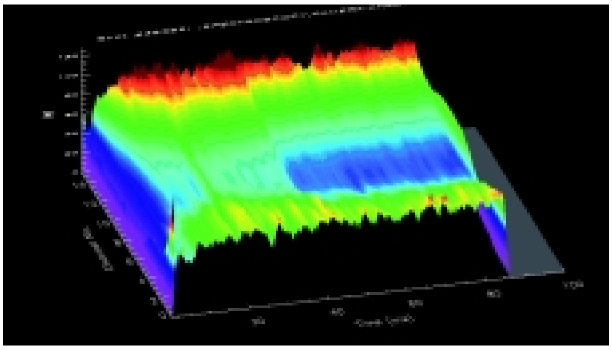
BLINE, an object orientated vacuum magnetic field line tracing code with real time stereoscopic display of field lines and



(Top) High Power, High Frequency DC block for earth isolation of the H1-NF Heliac and an ICH transmitter. The device serves to transmit 250kW of RF power from the transmitter to the heliac and provide up to 3kV of DC isolation between earths (Bottom) David Anderson and Michael Blacksell of the School's Electronics Unit, working on the DC block



False colour topographic plot showing the interferometer phase shift (proportional to plasma density) as a function of laser beam position in the plasma (Channel No.) and time (horizontal axis) during a resonantly heated hydrogen discharge at 0.5 T. (above) False colour topographic plot showing the time evolution of the hollow ion temperature profile during an rf generated argon discharge at low field (0.2T) (below)



conductor elements was implemented this year. A computational step rate of 50,000 steps/second was achieved integrating along magnetic field lines while maintaining a stereo display refresh rate of 40 frames/second on a personal computer. A perturbation calculation was added to allow optimisation of additional windings by simulated annealing at rates faster than one iteration per second. This is applicable to detailed error field calculations, flexibility windings such as the helical core in the H-1 heliac, or in new designs using advanced configurations. A Compact Disk or downloadable file (http://rsphysse.anu.edu.au/prl/bline) containing H-1 magnetic field data and the interactive tracing program in web browser format has been completed. This will prove useful to collaborators who need to understand the H1-NF magnetic geometry in detail. *(B.D. Blackwell, B.F. McMillan, A. Searle and H.J. Gardner*)

Plasma Diagnostic Systems

Diagnostics for Transport and Turbulence Studies

Several new diagnostics have been developed to study plasma transport, instabilities and turbulence in the H1-NF. Specific examples include a Thomson scattering diagnostic, electrostatic and magnetic probes, and a 20-channel correlation spectroscopy diagnostic.

A multi-channel Thomson scattering diagnostic is being set up on H-1 to measure the electron temperature and electron density profiles. This diagnostic will complement the multi-channel spectroscopic diagnostic in the higher electron temperature plasma (> 100 eV). The system is based on a 10 J 15 ns Ruby laser (currently being commissioned). The detection system uses a sensitive (>10% quantum efficiency) image intensified two-dimensional (512x512) CCD array camera (Roper Scientific) which allows simultaneous measurements of spectra of the laser light scattered from more that 10 radial regions in the plasma.

A 20-channel spectroscopic diagnostic (visible range) capable of measuring the electron temperature and the electron density mentioned above, is easily converted into a 10x10 channel correlation spectroscopy diagnostic capable of characterising longer wavelength (wave numbers < 8 cm^{-1}) fluctuations of electron density. Fluctuations in the plasma density and electron temperature both contribute to the fluctuations seen in the measured intensity of spectral line emission. By cross-correlating chord-average line intensities it is possible to obtain spatially localised fluctuation intensity, frequency spectra and the fluctuation correlation lengths. First results confirm the earlier observation using Langmuir probes of the m=1,2 and 3 poloidal modes dominating the plasma in the low confinement mode in H-1. This diagnostic complements the microwave (~140 GHz) scattering diagnostic in the long wavelength range.

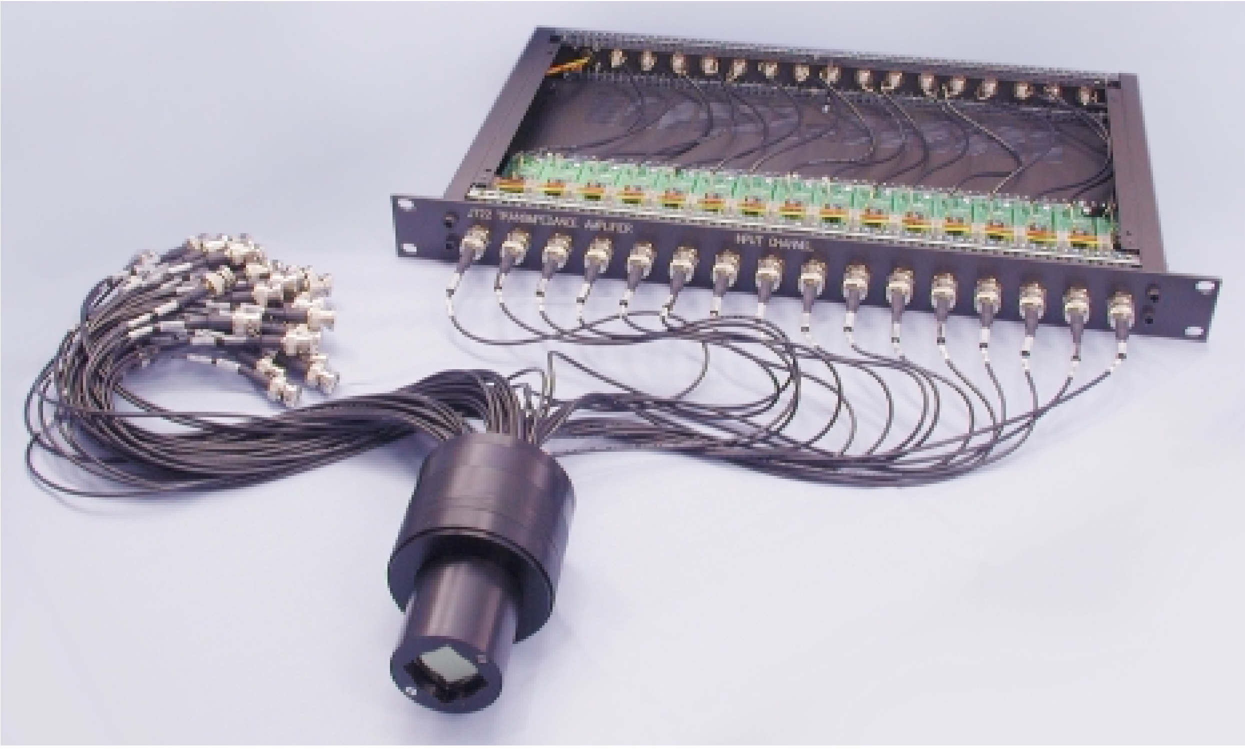
Several novel probe techniques have been developed and tested on H-1 to estimate radial particle transport. A new radial paddle (or Mach) probe has been installed to measure radial ion drift or transport in the plasma. A revised theory of the unmagnetised Mach probe has been suggested which extends the original Bohm theory towards the high ion temperature range. The radial Mach probe has been used in combination with 4 triple probes and the results are combined in a model, which allows an experimental evaluation of the electron and ion particle fluxes (including time-dependent components). *(M.G. Shats, W.M. Solomon, H. Punzmann, A. Gough)*
http://rsphysse.anu.edu.au/~mgs112/html/turbulence

Interferometry

Following modification in 1999 for operation at 743 microns wavelength, the far-infrared scanning interferometer has been operated reliably to provide plasma density profile information. The system has been tested at high magnetic field strength, and new software developed for automatic numerical phase demodulation and archiving under the MDSplus data system. The acoustically noisy high-speed air turbine for rotating the scanning grating has been replaced with a quiet computer-controllable electric motor drive. Plans are well advanced for installation of additional plasma views that will aid reliable tomographic reconstruction of the plasma density distribution. Greater viewing access to the plasma for the FIR system has necessitated relocation of the swept frequency 2 mm interferometer to an adjacent port. *(J. Howard, N. Gyaltson and S. Collis)*

Spectroscopy

This year the focus has been on both the development and application of advanced diagnostic instrumentation based on the MOSS spectrometer. This instrument, which has been patented by the ANU, is a modulated fixed-delay Fourier transform spectrometer based on solid electro-optic birefringent components. It is used for polarisation and Doppler spectroscopy of transition radiation from neutral atoms and from ions. Some of the earlier work on MOSS was this year recognised with an



One of the 16 channel transimpedance amplifiers of the the tomographic MOSS system built by the School's electronics unit (above) The tomographic MOSS system with some of its creators (below)

invited presentation to the "13th APS Topical Conference on High-Temperature Plasma Diagnostics" in Tucson Arizona.

The MOSS program for 2000 is summarized below. More information about the MOSS spectrometer and related technologies can be found at **http://rsphysse.anu.edu.au/prl/ MOSS.html**

- A 16 channel MOSS camera for Doppler spectral imaging studies of plasma dynamics and transport has been installed and operated. First studies of ion transport using modulational techniques that take advantage of the good time-resolution afforded by MOSS have been undertaken.

- The tomographic MOSS system (ToMOSS), which is based on a rotatable platform that supports an array of 55 lens-coupled optical fibres that view the H-1 plasma, has been installed. The light signals are transported to a 2-D MOSS camera for spectral processing prior to acquisition by the H-1 digital CAMAC data system. Tomographic reconstructions are now routine.

- A benchtop system for Zeeman spectroscopy is being constructed. The instrument, which will be trialled in the Faculties, has application for sensitive and fast measurement of current profiles in large tokamaks (e.g. DIII-D) as well as in solar astrophysics.

- The multiple fixed delay Spread-spectrum Optical Fourier Transform (SOFT) spectrometer (an extension of the MOSS idea) has been successfully operated and first results reported. This system allows time-resolved high-resolution study of spectral lineshape details. The information is encoded on a number of discrete carriers (channels) in the temporal frequency domain.

- Intra-vacuum lens-coupled optical fibres for MOSS/SOFT study of ion distribution functions have revealed important information pertaining to ion heating in H-1NF. The results are being prepared for publication. *(J. Howard, F. Glass, C. Michael, A. Danielsson, B. Blackwell, J. Wach and M. Blacksell)*

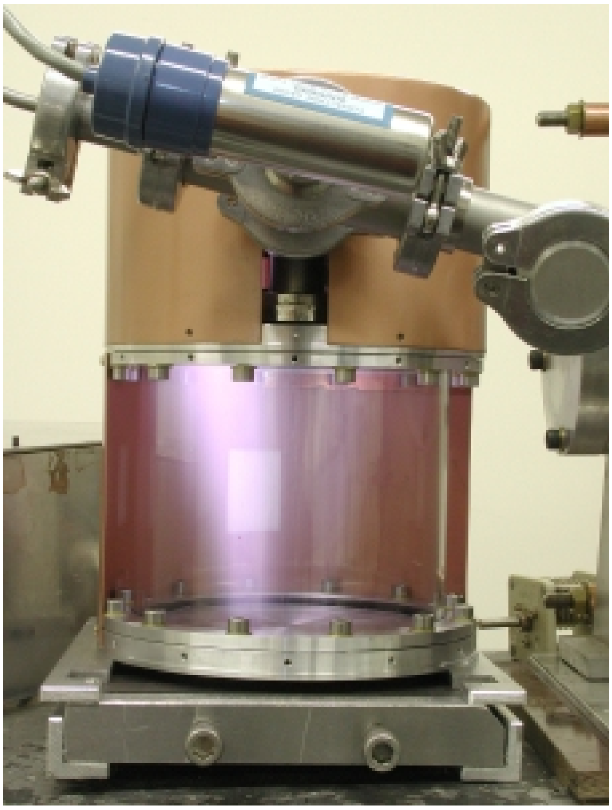
Plasma Antennas and Wireless Communications

The Defence Science and Technology Organisation (DSTO) has funded three contracts for the development of a plasma antenna. The first contract in 1997-1998 was to investigate the feasibility of the plasma antenna for radio frequency communications and radar, and the second contract (1998–1999) to develop an HF plasma antenna concept demonstrator. These contracts were successfully completed and two concept demonstrator antennas delivered to the DSTO in May 2000 which is currently carrying out testing. In the third contract, 1999-2000, a concept demonstrator microwave plasma lens was completed in June. The lens has formed the basis of a new contract with DSTO which furthers the applications of the plasma antenna in the microwave range by using the refractive index gradient of a plasma to deflect a 35GHz microwave beam.

The Plasma Research Laboratory was successful in attracting further contracts and grants in the year 2000. These include a SPIRT grant won in collaboration with CEA Technologies, ACT, to develop the HF plasma antenna for ship-borne communications and radar, and a contract for a post-graduate scholarship from Motorola, USA, for the investigation of plasma switches for mobile phones. A RIEF grant was obtained for $150,000 to purchase state-of-the-art equipment to support work on plasma antennas and wireless communications. This will be used to test critical communications and radar-relevant parameters for the plasma antenna, and novel communications schemes at VHF. The equipment will also support education in radio-frequency and wireless, following the inception of a new practice-based wireless course in the curriculum of the Faculty of Engineering and Information Technology. The lecture notes are available at http://wwwrsphysse.anu.edu.au/~ggb112/course/introduction.html *(G.G. Borg, P. Linardakis, L. Lungu and J.H. Harris)*

Australian Fusion Research Group (AFRG) Collaborations

The AFRG meets regularly to coordinate a wide range of collaborative activities on H-1NF involving both professional staff and postgraduate students at universities around Australia. These programs are summarised below. In the period under review, the Group undertook an intensive undergraduate level course in plasma physics in order to expose potential graduate students to the field. This course is seen to be necessary as there are only three universities in Australia that teach formal courses in plasma physics. The course was run for the first time in 2000.



The plasma lens in operation. The gradient in the refractive index of the plasma deflects a microwave beam

Digital Signal Processing (Central Queensland University)

The use of wavelet transforms in time-frequency analysis of plasma diagnostic data has been investigated. The plasma density and potential fluctuations from the Langmuir probe diagnostics were analysed using wavelets, and their effect on particle transport was studied. This work is led by Central Queensland University, and funded by an AINSE travel grant. *(X-H. Shi, J. Boman [CQU] and M. Shats)*

Plasma Theory (Flinders University)

A resistive MHD stability and spectral code, SPECTOR-3D, is being developed for 3D helical configurations to be applicable to stellarators and, in particular, to H-1NF. The collaboration which began in 1999 was funded by an AINSE travel grant in 2000. *(R. Storer [Flinders University] and H.J. Gardner)*

Soft X-ray Measurement System (University of Canberra)

The housing for the 16-channel X-ray detector, which has now been constructed, comprises a stainless steel cylinder with a detachable beryllium-foil covered slit at one end to provide a light-tight view of the plasma. The other end supports the mounting for the detector chip and its amplifiers, with a light-tight labyrinth to allow cable egress. The detector assembly has been mounted above the plasma and slightly outboard to afford a view along the long cross-section of the plasma. It has been placed as close as practicable to the multi-channel interferometer to allow correlation between density and temperature measurements. Currently 8 of the 16 channels have been connected; these eight will view the plasma along the central chord, 3 inboard chords and 4 outboard. Currently external circuitry is being constructed. Measurements of the soft X-ray flux will allow calculation of plasma pressure, electron temperature and the effects of impurities. *(B.D. Blackwell and A.D. Cheetham [UC])*

High Voltage Modulator for the MOSS Camera (University of Canberra*)*

Consistent with efforts to use commercially available hardware wherever possible, the MOSS drive circuitry is based on standard stereo audio amplifiers and high voltage, low-loss step-up transformers to excite the essentially capacitive crystal load. Important progress was made in developing and testing a comprehensive network model that describes the electrical behaviour of the MOSS drive circuitry. The model has been used to tailor drive requirements to suit specific MOSS applications. *(J. Howard and A.D. Cheetham [UC])*

Laser Induced Fluorescence (University of Sydney)

A laser induced fluorescence system is being developed for measurement of edge electric fields in the H-1 heliac. Following grants from both Research Infrastructure Equipment and Facilities (RIEF) and Australian Research Council large grant schemes, Dr Peter Feng was appointed to a three-year position with the University of Sydney to undertake this work. This work is being coordinated by the University of Sydney. *(J. Howard, B.W. James and P. Feng)*

Fibre Sensors (University of New England)

The University of New England developed novel optical fibre sensors and bolometers for electric field and thermal measurements in the edge and body of the H-1NF plasma. Their insulating nature and immunity to high voltage and electromagnetic noise makes these devices particularly attractive for plasma work. This year brings an important phase of this work to a conclusion with Vernie Everett now in the process of writing up the results for his PhD thesis. *(J. Howard, B.D. Blackwell, J.H. Harris; V. Everett, G.B. Scelsi and G.A.Woolsey [UNE])*

Space Plasma and Plasma Processing Group

The SP^3 Group is primarily concerned with the basic physics of gaseous discharges and their application in the processing of thin films. Plasma modification of surfaces is one of the fastest growing areas of scientific research and industrial development in the world. Highlights of the current research program are described in the following paragraphs.

Optical Waveguides

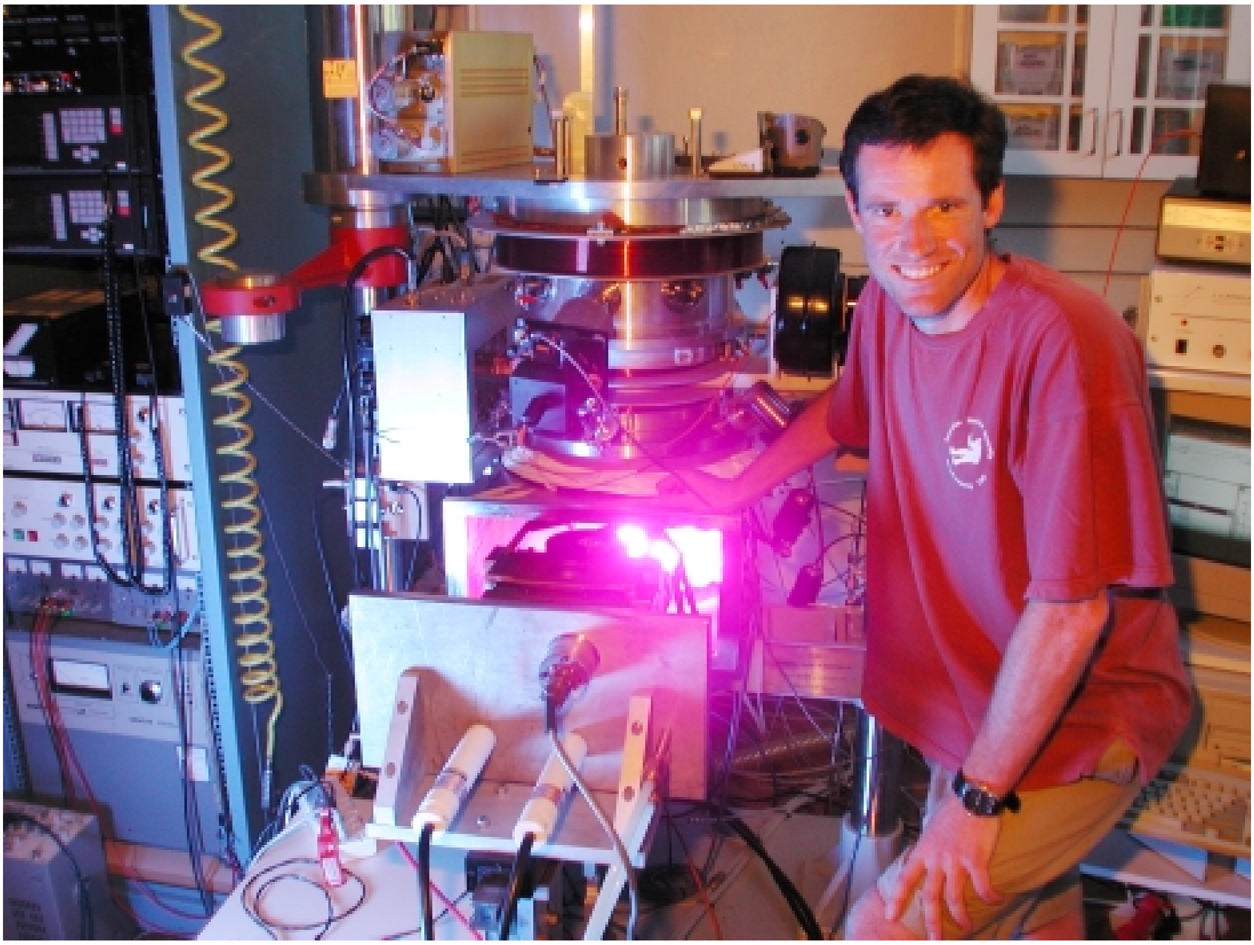
In collaboration with Professor John Love from the Optical Sciences Centre, the Group was the first in Australia to design and fabricate silica planar waveguides. This work has been continued with the improvement of the fabrication of passive splitters for use in Local Area Networks. A new direction has been opened using the Helicon Activated Reactive Evaporation (HARE) for doping of silica films with germanium, for applications in active and nonlinear devices. The Group has reported the first UV-induced refractive index change in germano-silicate glass containing no detectable level of hydrogen. This work is continuing with the design and fabrication of multimode waveguides, involving the deposition and etching of thick silica films, and with further investigation of doping of silica for photosensitivity effect. *(R.W. Boswell, K. Gaff, R.A. Jarvis and J.D. Love[OSC])*

Helicon Assisted Reactive Evaporation (HARE)

HARE is a plasma assisted reactive evaporation system that combines an evaporation source (electron beam) and a high density helicon plasma source in a configuration where the evaporant material is transported through the plasma source. This technique allows deposition of a large variety of materials without requiring the handling of hazardous chemical precursors. The performance of the system has been greatly improved by the installation of a 3-crucible electron beam system from JEOL allowing the independent evaporation of silicon and two dopants. Present research is focussing on the hydrogen free films and the machine conditions that allow its growth. *(R.W. Boswell, K. Gaff and S. Hatch)*

Retarding Field Energy Analyser and Multiple Retarding Field Energy Analyser

The helicon system "Chi Kung" which comprises a 15 cm diameter pyrex source tube 30 cm long attached to a 30 cm diameter, 30 cm long aluminium diffusion chamber, is a research reactor for basic helicon and plasma phenomena. A retarding field energy analyser has been used on "Chi Kung" to test its responses and to start an experimental design for the 9 channel multiple retarding field energy analyser before it is placed into the H-1NF. The first experiments concerned an expanding



Keith Gaff with the Helicon Activated Reactive Evaporation (HARE) system. An open air plasma?!

plasma, as there remains considerable interest in the evolution of the ion energy distribution function. The self-consistent field created by the gradient in the axial density can be considerably greater than the difference between the plasma and floating potentials. A large oscillating rf potential was also detected by floating Langmuir probes, together with a two-humped ion energy distribution function. A number of models are being developed to extract the actual rf potential and eventually the rf field along the axis of the machine. *(C. Charles and R.W. Boswell)*

Three Dimensional and Stereo Data Visualisation Systems

A Robot Command Station is being designed and constructed for the remote operation of a mobile robot using a stereoscopic display system. As part of this command station, investigations into the processing of digital stereo video will be undertaken with particular emphasis on near real-time compression and transmission of this data.

Data visualisation plays an increasingly important role in interpreting scientific experiments and computer simulations. A considerable proportion of a research degree involves developing techniques to manipulate and view large sets of multi-dimensional data, and often this is difficult within the confines of a two-dimensional screen.

Demonstration systems were developed in collaboration with the ANU Supercomputing Facility. A large-scale system was sold to the Powerhouse Museum in Sydney where it is on public display and an even larger system installed in the new CSIRO Discovery Centre at the Plant Sciences building in Canberra. A system will soon also be operational in the Australian Defence Forces Academy, Canberra. Applications to virtual engineering design and data analysis are also being developed in the H-1NF. (*R.W. Boswell, H.J. Gardner and R.P. Hawkins*)

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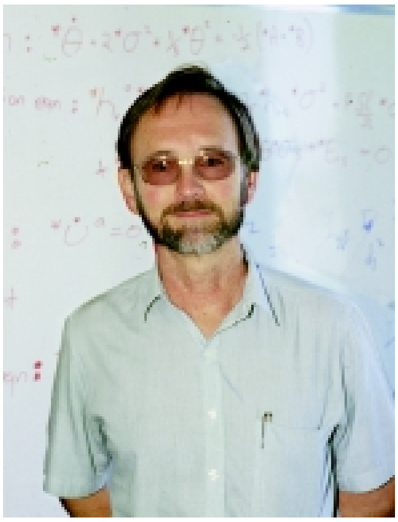
Theoretical Physics



Professor Robert Dewar
- Head of Theoretical Physics

http://wwwrsphysse.anu.edu.au/theophys

Research Summary

The study of physics involves the discovery of quantitative laws of nature and the elucidation of their consequences as they manifest themselves in complex ways. As we make sense of this complexity on each length and time scale, new "laws" emerge forming a hierarchy, from those describing the elementary particles on the smallest scales, through nuclear physics, atomic physics, condensed matter physics, plasma and fluid dynamics, astrophysics and finally, at the largest scale, cosmology.

Aspects of physics on all scales are covered in the research interests of the Department. Although the borderlines can be blurred, for convenience the research is reported under the headings of *Microscale Physics* (from the atomic scale downwards), *Mesoscale Physics* (assemblies of atoms into lattices and small structures where quantum mechanics is often still important) and *Macroscale Physics* (from the scales of everyday experience to those of the universe). Many mathematical and numerical techniques are common to all scales and the development of such knowledge provides a unifying theme throughout the activities of the Department.

The Department is host to the Australian National University Centre for Theoretical Physics (ANUCTP), a precursor of, and partner body in, the National Institute for Theoretical Physics, a consortium centred in Adelaide. The Centre is involved in a broad range of theoretical activities represented in the School and on the ANU campus.

Highlights of the ANUCTP activities this year were the 13th Physics Summer School on *Bose-Einstein Condensation: Atomic Physics to Quantum Liquids* held in January and organised by Dr Craig Savage and Dr Mukunda Das; the International workshop, *The Baxter Revolution* in February organised by Dr Murray Batchelor (School of Mathematical Sciences), Professor Vladimir Bazhanov and Dr Paul Pearce (University of Melbourne); and the workshop *Soft Condensed Matter: Physical and Biological Aspects* in October organised by Dr David Williams (Applied Maths).

Mesoscale Physics

Condensed Matter Physics

Density Functional Theory of Super-Phenomena

Density functional theory is now regarded as being a standard model for low energy physics, having a rigorous and well-defined structure. In the past three decades it has delivered very impressive successes in the study of normal states of matter. However, experience shows that at a low enough temperature the lowest energy state of a many body quantum system is not really a normal state. Inter-particle correlations in conjunction with statistics connive to form condensates, which exhibit super-phenomena (superconductivity and superfluidity). In the realm of density functional theory we have studied the occurrence of Fermi and Bose condensates, and have thereby obtained a pairing potential that sustains an order parameter due to broken symmetry. At the Hartree mean field level this theory has produced the well-known BCS results. *(M.P. Das)*

High Tc Superconductivity and Strong Electronic Correlations

Strong electronic correlations seem to influence the physical properties of solids resulting in peculiar anomalies. Using the Hubbard model we have studied the metal-insulator transition, various aspects of the normal state of high Tc super-conductors, and the effect of substitutional impurities for Cu within the CuO planes of high Tc materials. This investigation is of considerable benefit in gaining insight into both the normal and superconducting properties. *(M.P. Das)*

We are studying the isothermal compressibility and long-wavelength static density-density response function of a weakly correlated two dimensional electron gas in the weak degeneracy regime. Here the Fermi temperature and the physical temperature are comparable. Our preliminary results indicate that at low density of electrons the correlation energy dominates over the exchange contribution. *(M.P. Das, K.I. Golden and F. Green)*

The comprehensive investigation continues into the properties of the conducting phases of one- and two-dimensional electronic systems, using the non-Abelian density matrix renormalisation group (DMRG) method developed during last year. The method was successfully applied to several strongly correlated electron systems. In particular, in one dimension we studied the Kondo lattice model, the periodic Anderson model and the t-t'-U Hubbard model. In two dimensions, the Kondo lattice and the standard Hubbard model were studied, where work concentrated mostly on studying the stripe phases. This new non-Abelian DMRG method was applied to several other models in collaboration with Professor Anders Rosengren and Ausrius Juozapavicius (Stockholm) and Dr Alan Bishop (Los Alamos). *(M. Gulacsi and I. McCulloch)*

The central problem posed by heavy fermion materials is to understand the interaction between an array of localised moments (generally f-electrons in lanthanide or actinide ions) and conduction electrons (generally p- or d-band). This problem has been studied in low dimensional strongly correlated systems which are well described by the periodic Anderson models. We have used an analytical approach, based on non-Abelian bosonisation, showing that the effective interaction between the localised moments is of a ferromagnetic double-exchange type. Future work will be dedicated to determine exactly the phase diagram of the model. *(M. Gulacsi and H. Horn)*

Systematic analysis of the finite temperature properties of the Luttinger liquids has continued. Dr Miklos Gulacsi and Garry Bowen have developed a finite temperature non-Abelian Bosonisation method which was consequently used to calculate all asymptotic correlation functions and critical exponents at any finite temperature. This result allowed the momentum distribution function to be calculated. Analysing the property of the momentum distribution function, Dr Miklos Gulacsi and Meera Parish have established the fractional statistics corresponding to the elementary excitations of a Luttinger liquid. *(M. Gulacsi, G. Bowen and M. Parish)*

At present the nature of high-temperature superconductivity remains elusive, in spite of the fact that many novel models have been proposed. This problem was addressed by Dr Miklos Gulacsi and Raymond Chan using a technique, developed by themselves, based on an infinite order unitary transformation. In theoretical physics unitary transformations are used to get deeper insight into the physical phenomena, since the transformed Hamiltonians will reveal the appropriate independent subsystems. The transformation was successfully applied to the two and three band, two dimensional Hubbard models containing phonons. The effective spin and charge interactions were exactly determined. *(M. Gulacsi and R. Chan)*

Mesoscopic Systems

High field transport and noise in degenerate conductors still lacks a systematic theoretical description, despite its importance for microelectronics. We study a practical theory of nonequilibrium fluctuations in metallic mesoscopic systems, accounting for the dominant Fermi liquid behaviour of the electrons. The Pauli exclusion principle determines the electronic properties of a metal near equilibrium, right from the microscopic level to the bulk. Information on the carrier kinetics can be reliably obtained from the shot noise spectral density. Here we can obtain the nature of screening and the charge quantum of the carriers from the spectral density function. We are now using these ideas to investigate the fractional charge and fractional statistics of carriers in the fractional quantum Hall experiments. *(M.P. Das and F. Green)*

The 1956 Tassie model for incompressible oscillation of an inhomogeneous fluid is being extended from nuclear physics to the collective oscillations of Bose-Einstein condensates. *(L.J. Tassie)*

Resonant Solitons in Semiconductors

Applied research on dynamics of the resonant solitons in the excitonic spectral region of semiconductors has been continued. The main objective has been to demonstrate a possibility of tunable operation of the resonant soliton switches and logic gates near the optical communication wavelength (1.55 microns). Numerical investigation of the wavelength dependence of the resonant soliton switches has been performed. A number of semiconductor materials which allow tunable device operation near 1.55 microns have been identified.

The theoretical work has initiated a large-scale experimental effort to study ultrafast excitonic optical switches and logic gates. The prototype devices have been fabricated using GaAs/AlGaAs multiple quantum-well structures. Device characterisation using a modelocked Ti:sapphire laser is to commence shortly. *(N. Peyghambarian [University of Arizona] and I. Talanina supported by Phase I STTR Grant from the U.S. Air Force Office of Scientific Research)*

Mathematical Physics

We have continued our study of solvable models in statistical mechanics and related areas of mathematical physics. Since 1978 there has been a great deal of work in statistical mechanics on models on random lattices. This appears to have overlooked earlier work by W.T. Tutte on dichromatic polynomials, i.e. Potts models on random rooted planar maps. We have extended Tutte's work to non-separable maps to obtain a non-linear recursion relation for the partition function. We have solved three special cases exactly, and have verified from numerical studies that the system has a transition much like the regular lattice Potts model. One advantage of this model is that it should be possible to calculate the free energy and thermodynamic properties away from the phase transition.

An intriguing problem in combinatorics is that of counting "meanders", i.e. the number of distinct non-self-intersecting walks that cross a river 2n times, returning to the starting point. This can be expressed as a trace over an operator in the Temperley-Lieb algebra that has played such a significant role in the planar six-vertex and Potts model, so is in that sense a (rather simple) partition function. So far the problem has proved intractable: can this algebra provide a route to its solution? *(R.J. Baxter)*

The continuous version of Baxter's commuting transfer matrix method has been developed for conformal field theories with the extended W_3 symmetry. The results were applied to exact calculation of non-equilibrium transport properties for the quantum Brownian motion on a triangular lattice. An interesting connection of the results to the spectral theory of third order differential equation is also established. *(V.V. Bazhanov and A.N. Hibberd)*

Microscale Physics

Nuclear Theory

Hadron Physics

Work on the calculation of the electromagnetic corrections that need to be applied in the analysis of scattering data at low energies has now been completed and published. An analysis of the data to determine the hadronic phase shifts at low energies is continuing; the best method of treating the systematic errors is still being considered. New calculations on the extraction of hadronic parameters from the results of an experiment on the atom (pionium) in progress at CERN have been completed. *(W.S. Woolcock, G.C. Oades [Aarhus], G. Rasche and A. Gashi [Zürich])*

Light Nuclei

R-matrix formulas have been used to derive information about levels of ^{8}Be and reactions involving ^{8}Be. Data from the ^{4}He(α,p)^{7}Li, ^{4}He(α,n)^{7}Be, and ^{7}Li(p,α)^{4}He reactions and from $\alpha+\alpha$ elastic scattering were fitted, and a value obtained for the zero-energy S factor ^{7}Li(p,α)^{4}He: $S(0)$ = 58 keV b. Recent measurements and analyses of the ^{7}Li(d,α)an and ^{7}Li(p,γ)^{8}Be reactions, and calculations concerned with low-lying intruder states in ^{8}Be, were discussed with reference to *R*-matrix fits. A calculation of the width of the ^{12}O ground state due to ^{2}He emission has given an upper limit of 5 keV, much less than a recently published value of 340 keV. *(F.C. Barker)*

Data for the ^{9}Be(p, α)^{6}Li and ^{9}Be(p,d)^{8}Be reactions with proton energies up to 700 keV have been fitted using *R*-matrix formulae. The data include values of the astrophysical S factors and of the angular-distribution and analysing-power coefficients. *(F.C. Barker and Y. Kondo [Kyoto Women's University])*

R-matrix fits have been made to the deuteron spectrum following ^{6}He beta decay. *(F.C. Barker and Canadian group [TRIUMF, Simon Fraser University, University of Toronto])*

Antiproton-Deuteron Scattering

An analytic solution for the $\bar{\mathrm{p}}\mathrm{d}$ high energy elastic scattering amplitude has been derived using a harmonic oscillator wave function, with a D-state component for the internal wave function of the deuteron, within the framework of Glauber's approximation to multiple scattering theory. Fitting the experimental differential cross section for $\bar{\mathrm{p}}\mathrm{d}$ elastic scattering at 179.3 MeV, employing the $\bar{\mathrm{p}}\mathrm{p}$ scattering amplitude obtained from $\bar{\mathrm{p}}\mathrm{p}$ scattering experiments, permits the parameters of the elementary $\bar{\mathrm{p}}\mathrm{n}$ scattering amplitude at 179.3 MeV to be obtained. The results have been compared with other analyses. *(B.A. Robson and Zhang Yu-Shun [Institute of High Energy Physics, Academia Sinica, Beijing])*

Nuclear Fusion

The possibility of inducing the complete fusion of heavy nuclei has been a strong motivation in the quest to synthesise new nuclear species, especially superheavy elements. Work has commenced to understand the various approaches employed to describe the fusion of two heavy ions for energies close to or below the Coulomb barrier. Such approaches include semiclassical transport theories, incorporating both dissipative (frictional) forces and fluctuating (Langevin) forces, and quantum mechanical techniques associated with tunnelling through barriers and coupling to other nuclear degrees of freedom. *(B.A. Robson)*

Interacting Boson Model

In recent experiments, positive and negative parity bands in actinide nuclei were found to be in close proximity, which requires treatment of quadrupole and octupole degrees of freedom in collective models on an equal footing. This presents a formidable challenge for nuclear models due to both the increased number of parameters and much larger model spaces. As a first step towards this goal, we have carried out a mean field study of the *spdf*-boson model, deriving simple formulas for main spectroscopic observables (e.g. band excitation energies and electromagnetic transitions). For realistic choices of the Hamiltonian parameters, the ground state of the system is shown to remain axially symmetric, which considerably simplifies the mean field treatment. A systematic survey of excitation energies and electric transitions for one-phonon states is given, which will provide a useful guidance for detailed studies of negative parity states within the *spdf*-boson model using either numerical diagonalisation or projection techniques. *(S. Kuyucak and M. Honma [Aizu University])*

Atomic and Molecular Physics

Theory of Many-Electron Correlations in Solids

Ab initio calculations of many-electron correlations in solids became feasible recently with advent of high-performance computers and development of sophisticated theoretical methods. A promising computational scheme is the so-called GW approximation that takes into account the screening of the inter-electron interaction in the self-energy operator. Vertex corrections to the GW approximation in the form of the cumulant expansion are found significant and incorporated into the model. On this basis, the satellite structure in the ionisation spectra of solid carbon was simulated and found to be in excellent agreement with the recent experimental data from the electron momentum spectroscopy group at the ANU. Further correction of the theory using the T-matrix approach is now under consideration. This will allow the consideration of many-deuteron correlations in narrow band *d*-electron systems. *(A.S. Kheifets and F. Aryasetiawan [University of Lund])*

Theory of Multiple Atomic Ionisation

Multiple atomic ionisation following absorption of a photon or a knock out from a fast projectile is currently a very active field of atomic collision physics. Because of the pivotal role of the electron-electron correlations, these processes continue to receive considerable attention, both theoretically and experimentally. In previous years the theory of multiple atomic ionisation based on the convergent close-coupling method proved its success when applied to the two-electron ionisation of the helium atom. In the year 2000, the theory was expanded to include the helium atom in its metastable states and alkaline-earth atoms (Be and Mg). Predictions of the theory for the electron impact double-ionisation of helium, initially at odds with the experiments, were finally confirmed in a series of experiments at the University of Freiburg. Work on triple photoionisation from Be and Mg has been initiated. *(A.S. Kheifets, I. Bray [Flinders University] and A. Ipatov [St. Petersburg Technical University])*

Hydrogenic Atoms

Previous work using the dipole approximation for hydrogenic atoms has indicated that an eight-component theory developed by Robson and Staudte predicts different Balmer-α and Lyman-α spontaneous radiative transition probabilities than those given by the standard Dirac theory. The extension of this work to calculate the transition probabilities without making the dipole approximation, and also to calculate the so-called "forbidden" components, has now been completed. The results confirm that the eight-component and Dirac theories predict different transition probabilities for the components of the Balmer-a and Lyman-a lines. *(B.A. Robson and S.H. Sutanto)*

Spontaneous Coherence and Slow Dephasing in Quantum Systems

Evidence for deterministic randomness in quantum systems has been found in a collaborative venture between Chinese experimentalists and the ANU. This phenomenon is conceptually forbidden in modern quantum theory. Yet, the data support Kun's theory of spontaneous coherence, slow phase randomisation and extreme sensitivity in highly excited quantum systems. This demonstrates that a realisation of Wigner's dream, a theory for the transition amplitude correlations, has led us to a conceptual revision of modern understanding of microscopic and mesoscopic many-body systems. Further tests of Kun's theory will be carried out in China in 2001. *(S.Y. Kun, Wang Qi et al. [IMP, Lanzhou] and Li Zhichang et al. [CIAE, Beijing])*

Chemical reactions typically proceed through the formation of an intermediate molecular complex (IMC). For large molecules, the resonances of the IMC strongly overlap and many-body resonance states are ergodic due to the strong coupling between electronic, vibrational and rotational degrees of freedom. Conventionally, the decay of such an IMC is described within random matrix theory (RMT) which postulates the absence of correlations between the transition amplitudes. In sharp contrast, Kun's approach demonstrates a persistence of such correlations predicting a number of non-universal effects: (i) Coherent rotation of the IMC manifesting itself in quantum-classical cross-over in molecules. This effect has been observed in many isotope exchange chemical reactions. (ii) Micro-channel correlations — the effect has been observed in many unimolecular reactions. (iii) Coherence energy does not determine the reaction rate and application of the standard RMT can produce up to one order of magnitude error in the extracted rates. Accurate evaluation of the reaction rates is of great importance in numerous applications. *(S.Y. Kun)*

Modern quantum theory predicts that energy relaxation due to many-body effects is a sufficient condition for phase randomisation. In sharp contrast, Kun's approach demonstrates that a superposition of ergodic many-body configurations, whose spectrum obeys Wigner-Dyson statistics, can produce non-ergodic coherent states. This leads to a formation of stable highly excited coherently rotating two-electron one-hole molecules in quantum dots which distinctly affect the electron conductance. This offers the possibility to experimentally test the effect, and demonstrates its relevance for nanotechnology. A close analogy between artificial nano-molecules, nuclear molecules and similar effects in molecular systems is thoroughly elaborated. *(S.Y. Kun)*

Biophysics

Ion Channels in Biological Membranes

The KcsA potassium channel, whose crystal structure was determined recently, continued to be the focus of our Brownian/molecular dynamics simulation studies. We have improved on our initial simplified model of the KcsA structure by including all the atoms in the channel protein as determined from the x-ray diffraction. The molecular dynamics simulation results with the full structure were in broad agreement with those obtained with the simpler model. This justification of simpler models is important because full atomic simulations are very time consuming, and to make progress in relating structure to function, one has to reduce the complexity of the system. In the case of Brownian dynamics, there were slight improvements, e.g. the positions of the three potassium ions in the channel were in better agreement with those deduced from the X-ray diffraction experiments. Otherwise, the basic conduction mechanism deduced from the simpler model remained intact. *(S. Kuyucak, S-H. Chung and T.W. Allen [Chemistry, Faculties])*

The success of the simplified potassium channel structure in explaining the structure-function relationship has prompted us to investigate other channels whose structures are analogous to the potassium channel. Our first target was the calcium channel, which is very important biologically. While a lot is known about its conductance properties, its tertiary structure is poorly understood. Using the potassium channel structure as a template, we have constructed a model calcium channel that could explain most of its observed properties quite well. Among these are: the current-voltage curves, current-concentration relationship, block of monovalent currents by divalent ions, the anomalous mole fraction effect between sodium and calcium ions, attenuation of calcium current by external sodium ions, and the effects of mutating glutamate residues in the amino acid sequence. *(B. Corry, S. Kuyucak; S-H. Chung and T.W. Allen [Chemistry, Faculties])*

Macroscale Physics

Nonlinear Dynamical Systems

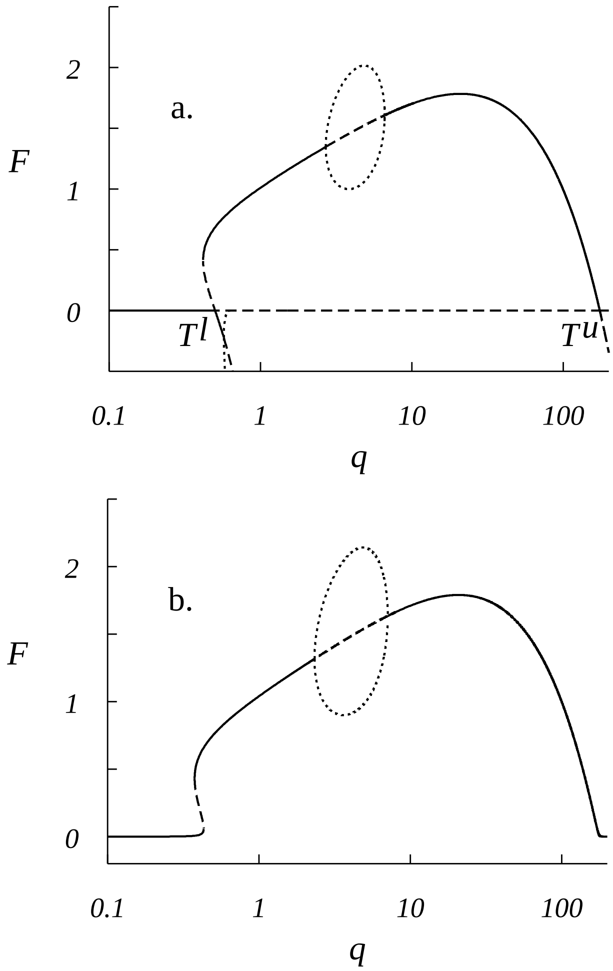
Singularity theory is a branch of mathematics that is concerned with the systematic enumeration, classification, and unfolding of degenerate bifurcations that typically occur in nonlinear dynamical systems. It provides a framework for describing predictively the emergence of abrupt changes, metamorphoses, oscillations, or "bad" behaviour from smooth, continuous, or "good" behaviour in dynamical systems. Often the onset of discontinuous action is ascribed to the propinquity of universal singularities such as pitchfork or Hopf bifurcations. Mapping of the topology of the critical surfaces formed when such singular points are unfolded is being developed as a new tool for the design, control and optimisation of systems. The aim is to calculate, visualise and animate the bifurcation manifolds of generic dynamical models that exhibit discontinuous phenomena. (See Figure below) *(R. Ball)*

Theory of Complex Fluids and Plasmas

The self-assembly of amphiphilic molecules, such as those of many therapeutic drugs, into micelle structures is often found to be a highly nonlinear dynamical process that is typical of a co-operative or autocatalytic mechanism. Under non-equilibrium conditions, multiple steady states and accompanying hysteresis are likely to be endemic to such systems. In this work singularity theory criteria were applied to enumerate and interpret the bifurcations occurring in a dynamical model for micelle formation, where nonlinear feedback is provided by a cubic autocatalytic rate term. Results to date show that hysteretic jumps between associated and dissociated states are controllable, thus giving us a molecular switching tool of potentially great power in applications such as control of drug action in vivo. Development of a project is in progress to demonstrate this effect with amiodarone, a potent cardiac antiarrhythmic, local anaesthetics such as cocaine and lidocaine (which also has antiarrhythmic action), and the psychotropic thiazine drugs. *(R. Ball and A.D.J. Haymet [Houston])*

A solid object like a bell supports a rich spectrum of normal modes of vibration. So too does a plasma equilibrium with a complicated shape, like that in a stellarator, with the added possibility that some eigenmodes may grow exponentially, signalling instability. In fact, the spectrum of ideal magnetohydrodynamic (MHD) pressure-driven (ballooning) modes in strongly nonaxisymmetric toroidal systems is singular, making it difficult to analyse numerically. The semiclassical (WKB) approximation is potentially an important tool for developing a qualitative understanding of this spectrum if we can adapt it to handle the singularity problem. We argue that reflecting boundary conditions at a *k*-space cutoff provides an appropriate regularisation for comparison with numerical eigenvalue calculations. This boundary condition makes ray tracing for the WKB ballooning formalism a chaotic Hamiltonian billiard problem. That is, we have a classical application of quantum chaos theory. The minimum number of Fourier basis functions for resolving localised ballooning modes with a global eigenvalue code has been estimated from the Weyl formula in the case of a strongly unstable plasma equilibrium in the H-1NF helical axis stellarator. *(R.L. Dewar, P. Cuthbert and R. Ball)*

Work is continuing on developing and analysing dynamical models that emulate transitions between low and high confinement states (L-H transitions) and associated periodic behaviour in confined plasma systems such as H-1NF. Singularity theory methods have been used to resolve a subtle case of overdetermination in existing published models, and to clarify the role of viscosity and diffusivity and a symmetry-breaking term in the onset, evanescence and extinction of discontinuous and oscillatory action that results from the coupled evolution of shear flow and turbulence. The smooth traversal of parameter space provided by this approach gives qualitative guidelines for controlling access to H-mode and oscillatory regimes. *(R. Ball and R.L. Dewar)*



(Top) The bifurcation diagrams for the new improved BD model emulate for the first time all of the major dynamical features of L-H transitions. (Bottom) Magnetic Islands in the H-1NF Heliac

The behaviour of magnetic islands at fusion relevant plasma pressures is of much interest for low shear stellarators such as the H-1NF Heliac. On the one hand, the lack of significant shear promises that island widths near low order rational values of the rotational transform could be very large and even catastrophic for plasma confinement. On the other, several stellarator experiments have been predicted to exhibit a property of “self-healing” with plasma pressure where the island width reduces to zero before changing sign. The objective of this project is to investigate this phenomenon for the H-1NF and to compare computer simulation with experiment. Because of the extremely three-dimensional, and bean-shaped, nature of the H-1NF magnetic field, the HINT equilibrium code, used for this study, has needed to be improved in speed and accuracy.

The previous year has seen more progress in the development of the HINT code and convergence studies of previous results have been undertaken. We feel that we are close to an answer to the question of whether, or under what conditions, self-healing exists in the H-1NF. *(H.J. Gardner and S.S. Lloyd)*

Dimensional MHD Resistive Stability

The development of a fully three dimensional resistive magneto hydrodynamic (MHD) stability code was commenced during the year. When completed this code will be applied to model large scale mode structures observed in the H-1NF and other fusion experiments. It will, hopefully, also be useful in the design of future advanced stellarators. *(H.J. Gardner and R.G. Storer [Flinders])*

A book aimed at honours undergraduate, or postgraduate level has been embarked on to give an overview of mathematics, not only for mathematicians who wish to know something outside their own speciality, but also for physicists, engineers, teachers and others with a serious interest in mathematics. All chapters have now been written and the final revision and co-ordination is well advanced. *(W.A. Coppel)*

Cosmology

We have continued work on the investigation of Isotropic Singularities (IS) in cosmological models. The IS project is an examination of a subclass of Big Bang-type initial cosmological singularities which have an associated conformal structure that is regular. Our recent work has centred on discovering a characterising feature of perfect fluid space-times which admit an IS. We have shown that, contrary to expectations in the literature, the Weyl tensor cannot be a characterising feature. We are currently making significant progress on this problem using new approaches. *(G. Ericksson and S.M. Scott)*

We also used the abstract boundary (a-boundary) construction of Scott and Szekeres to reanalyse the classical singularity theorems of Hawking, Penrose *et al*. In the last year we have proven a significant new a-boundary singularity theorem for maximally extended, strongly causal space-times. We have continued extending and generalising that theorem to incorporate the distinguishing causality condition. At the same time, new research into the stability of a-boundary essential singularities and the invariance of classification of a-boundary points under conformal changes of the metric has begun. *(M. Ashley, J. Beem [U. Missouri - Columbia] and S.M. Scott)*

Collaborative work has continued on a scenario for the formation of the universe by the fragmentation of macroscopic superstrings. *(L.J. Tassie and P. Brosche [Bonn])*

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