Research Accomplishments



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Research Accomplishments



Professor Stephen Hyde -Head of Applied Mathematics



http://rsphysse.anu.edu.au/appmaths

Applied Mathematics

Colloid, Surface and Polymer Science. Chemical engineering. New frontiers of Physics and some Biology too

Research Summary

Despite the current gloom enveloping Australian academia, induced largely by politicians, research at Applied Maths continues at full pace. The year has been an almost embarrassingly successful one on the home and international fronts. Research highlights are listed below. In tandem with those results, earlier this year we received a long-needed boost of about 25% in funding from within the University via the largest individual grant from the Institute-wide Performance and Planning Fund. The funding increase has allowed us to set up a nominally new research area, "mesoscale physics". The program is a natural extension of our work in the twin areas of self-assembly of molecular materials and transport in porous media, and seeks to move beyond the traditional domain of condensed matter physics into complex real world materials such as rocks and wood. These offer some formidable obstacles to hard scientific analysis: they are often spatially disordered, and are structured at a range of length scales, from Ångströms to microns. The first stage of this program – already underway – is to develop quantitative indices for characterisation of the topology and geometry of these structures. The work is strongly collaborative, with Professor Steve Cox in Geology and Dr Phil Evans in Forestry. We now have - for the first time in many years - the financial means to attract the best young researchers in this new interdisciplinary area. That effort is an add-on to our usual preoccupations: intermolecular forces, self-assembly of soft matter, and novel materials, that have contributed handsomely to our research output this year. Read on.

Surface Chemical Physics

Surface Phase Transitions of Near Frozen Liquids on Mica

Films of n-octadecane and n-hexadecane adsorbed on mica surfaces from vapour close to their bulk melting points (Tm) have been studied in a Surface Force Apparatus. The mobility and thickness of the adsorbed n-alkane films are found to undergo a transition a few degrees above T_m. We suggest that the adsorbed films undergo a transition to a more solid-like structure, akin to the postulated "surface freezing" or "surface ordering" of long-chain liquid n-alkanes.

Experiments are also being carried out with neo-pentanol and menthol. Unlike the case with long-chain alkanes, no freezing of liquid menthol is ever observed. It is likely that the difference is due to differences in nucleation of the solid phase at the vapour-liquid interface. The mica-liquid interface hinders nucleation of the solid phase with all liquids. Neo-pentanol appears initially to condense as a liquid, but often very rapid growth of the solid phase takes over, possibly due to direct nucleation from the vapour. (H.K. Christenson, M. Kohonen, N. Maeda, Y. Qiao)

Preparation and Characterisation of Fluorocarbon Surfaces for Force Measurements

Very hydrophobic heptadecafluoro-1,1,2,2,-tetrahydrodecyltriethoxysilane (FTE) surfaces have been prepared in various ways. Langmuir-Blodgett deposition at a low surface pressure yields an amorphous surface that is smooth homogeneous and has optimal hydrophobicity and good stability, whereas deposition at higher pressures give rougher surfaces with excess material. Adsorption from CHCl₃ gives smooth surfaces with large amounts of loosely held material that contributes to a larger contact angle hysteresis and lesser hydrophobicity. Adsorption from the neat fluorosilane yields a surface that is significantly less stable and less hydrophobic than the other surfaces. (H.K. Christenson; T. Ishida, [Joint Research Center for Atom Technology, National

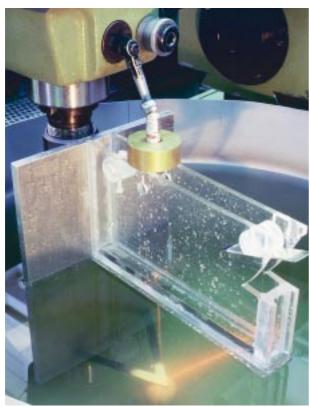
Institute for Advanced Interdisciplinary Research, Tsukuba, Japan]; S. Ohnishi, V.V. Yaminsky)

Capillary Condensation between Rinsed Mica Surfaces

In previous studies of capillary condensation of water between mica surfaces using the Surface Force Apparatus (SFA) it has not been possible to obtain agreement with the Kelvin equation. We have now carried out such experiments with mica surfaces that have been rinsed in dilute acid solution prior to mounting in the SFA. Unlike previous experiments, the refractive indices of water condensates between such surfaces are equal to that of bulk water and no visible deposits of involatile material remain upon evaporation. The equilibrium meniscus curvatures of the condensates agree with theoretical values calculated from the Kelvin equation. (*H.K. Christenson, M. Kohonen*)

Wetting and De-wetting Dynamics

The kinetics of capillary rise in glass capillaries of water, ethanol and mixtures thereof, have been studied by a high speed imaging technique. To adequately describe the experimental data a rate dependent dynamic contact angle has to be added to the Washburn-Lucas equation. This result is discussed in terms of a molecular friction coefficient at the front of the liquid flowing over the substrate. The kinetics of wetting and de-wetting of a glass surface by an aqueous solution containing the polyoxyethylene surfactant, $C_{18}OE_{84}$, has also been investigated. An overshoot of the liquid occurs before relaxation towards the equilibrium height. At concentrations well below and above the critical micellar concentration (CMC) of the surfactant the overshoot is small, while it is more pronounced in a range of intermediate concentrations (close to CMC). The kinetics of the



The worlds largest Atomic Force Microscope, set up in a tank of glycerine in the School's Mechanical Workshop, to test the macroscopic behaviour of the device

relaxation towards the equilibrium height also depends on concentration, with an increase in the relaxation rate at concentrations above CMC. The effects are due to a reduced (non-equilibrium) adsorption at the liquid/vapor interface. A 'pinning effect', that leads to an abrupt cessation of capillary rise, is discussed in terms of surfactant adsorption close to the three-phase line at the solid/vapor and solid/liquid interfaces. (A. Hamraoui [Centre de Recherche en Modélisation Moléculaire Université Mons-Hainaut, Belgium]; K. Thuresson, T. Nylander [Physical Chemistry 1, Lund U., Sweden,]; V.V. Yaminsky)

Adsorption Mechanisms of Dynamic (De-)Wetting Transitions: Principles and observations

Adsorption deposition by retraction from solution explains wetting/dewetting transitions induced by cationic surfactants on silica and mica surfaces. The theory of the hydrophobic phenomenon that follows in terms of values of surface pressure and adsorption has been extended from equilibrium situations towards kinetic effects. To confirm the underlying molecular mechanisms we have carried out ellipsometric studies of Cetyltrimethylammonium Bromide (CTAB) adsorption. (V.V. Yaminsky; K. Eskilsson, [Institute of Surface Chemistry, YKI, Stockholm])

Marangoni Effects in Spreading and Deposition of Nanoparticles from Drying Solvents

During preparation of nanoparticle films, complex condensation figures of two- and three-dimensional colloidal crystallisation may develop by interfacial instabilities. The Marangoni effect, responsible for the fractal structures of these colloidal aggregates, is due to surface tension gradients, induced by local cooling and/ or surfactant concentration gradients in the evaporation process. Macroscopically uniform nanoparticle layers self-assemble by retracting the substrate in an atmosphere of the solvent vapour maintained close to saturation. Surfactant-induced Marangoni instabilities are suppressed in micellar solutions compared with pure water. Layers of nanoparticles with uniform optical density over the entire area of the substrate have been prepared by slow solvent evaporation, that can be transferred without violation of the structure onto hydrophobic and hydrophilic surfaces using adapted Langmuir-Blodgett techniques. (V.V. Yaminsky; L. Motte, M. Maillard, M-P. Pileni, [Université P et M Curie Laboratoire, Paris])

Bridging Forces between Silica Surfaces in Cationic Surfactant Solution

Long-range hydrophobic forces observed between silica surfaces in solutions of cationic surfactants are due to bridging between the surfactant-polyelectrolyte complexes. The effect explains the "hydrophobic attraction" observed in such systems. (M. Persson, P. Claesson [Institute of Surface Chemistry YKI Stockholm]; V.V. Yaminsky)

Active Control of Liquids on Sub-millimetre Scales

Methods have been demonstrated for pumping and positioning of liquids on sub-millimetre scales using surface pressure gradients. This is achieved using a redox active surfactant. (B.S. Gallardo [Dept. Chemical Engineering and Materials Science, U. California]; V.K. Gupta, [Dept. Chemical Engineering, U. Illinois]; D. Eagerton, L.I. Jong, R.R. Shah, N.L. Abbott, [Dept. Chemistry, U. Newcastle]; V.S.J. Craig)

Dissolved Gas: Its Influence on Interactions in Aqueous Media

The effects of dissolved gas, surface approach velocity, and neutron irradiation on the measured interaction between hydrophobic surfaces has been studied. Each of these parameters was found to affect the magnitude of the force. The results are consistent with film instabilities playing a role in the long-range hydrophobic attraction. The mechanism by which restriction enzymes cut DNA has been resolved by extensive experiments as a function of salt, salt type and concentration and depends on dissolved gas and hydrophobic cavitation. The surprising result is that the co-ion and buffer co-ion are crucial determinants of activity. (V.S.J. Craig; B. Norden [Goteborg U., Sweden]; B.W. Ninham; R.M. Pashley [Chemistry, The Faculties])

Adhesion and Deformation of Polymers

Adhesion measurements between a range of substrates have been obtained using a commercial atomic force microscope. The results indicate that the geometry of interaction and the load applied between the interacting surfaces are critically important in determining whether an elastic or plastic type of interaction is seen. (S. Biggs, M. Reitsma [Dept. Chemistry, U. Newcastle]; V.S.J. Craig)

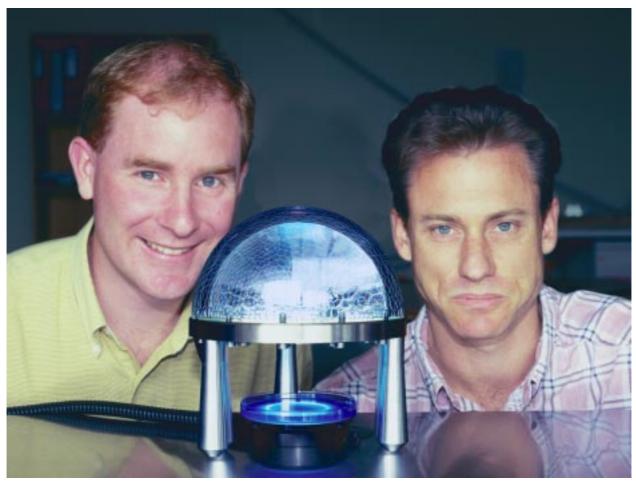
Adsorption Kinetics of a Cationic Surfactant to the Silica-Water Interface

The adsorption kinetics of CTAB to the silica-water interface was investigated using optical reflectometry. Analysis reveals that the adsorption process is cooperative above the critical micelle concentration, indicating that micelles adsorb directly to the silica-water interface. At the critical surface aggregation concentration $(0.6 \pm 0.05 \text{ mM})$ adsorption proceeds slowly in the absence of salt and takes hours to reach an equilibrium value. At all other concentrations and when salt is present, adsorption is complete within minutes. (*V.S.J. Craig; R. Atkin, S. Biggs [Dept. Chemistry, U. Newcastle]*)

Dynamic Measurements Using Atomic Force Microscopy

The hydrodynamics developed as a sphere is driven towards a flat surface have been investigated experimentally using an atomic force microscope (AFM). The measured force in a range of viscous liquids is compared with theoretical predictions and excellent agreement is found at separations of >100 nm. At smaller separations the measured force is less than predicted due to the onset of slip at the surface.

A commercial AFM has been modified to enable the stiffness of interaction between surfaces to be measured concurrently with the surface forces. The stiffness is described by the rheological phase lag between the AFM tip and a driving oscillation of the substrate. Silica surfaces bearing adsorbed polymers and surfactants have been studied. (V.S.J. Craig; S. Biggs, S. Notley [Dept. Chemistry, U. Newcastle])



Two Tims, Senden and Sawkins, with their spherical bubble morphology chamber

Lifshitz Theory of Molecular Interactions

By making use of the generalised multipolar gauge it has been shown that the matrix elements of the magnetic moment operator are independent of gauge origin for electromagnetic fields that are non-uniform in space and non-constant in time. This extends a previously published derivation and gives for the first time a completely general proof of a contention made many years ago by Van Vleck. (*A.M. Stewart*)

Charged and Hydrophobic Surfaces in Aqueous Solvents

Many of the remaining fundamental problems in colloid science are related to our inability to describe accurately specific interactions and processes involving solutes in the water solvent. Recent advances in molecular level simulations have furnished correlation functions and potentials of mean force for ions in aqueous solution. In the case of hydrophobic interactions, again there have been recent advances that provide simple analytical methods for the description of small solutes. During this year we established a formal basis for the technique and we have also improved the accuracy of simulated potentials and double layer calculations.

Work on hydrophobic solutes was initiated in Canberra this year, with a view to obtaining information on the transition between the small solute behaviour and the macroscopic surface tension of water. Initially we are investigating this transition in a molecular-level simulation. (S. Marcelja; A. Lyubartsev [Stockholm U.]; R. Kjellander [Goteborg U.]; A.S. Barisic; R. Sok [UNSW])

McMillan-Mayer Theory of Aqueous Electrical Double Layers

We consider the formal task of reducing the problem of electrical double layers in aqueous solvent to a simpler system where ions interact with other ions and with surfaces via the potentials of mean force. The exact mapping is achieved with a nonuniform fluid version of the McMillan-Mayer transformation. The results indicate the additivity of short- and long-range effects in ion density and pressure, and elucidates the basis for commonly used approximations. (*S. Marcelja*)

Flocculation of Hydrophobic Colloids

A systematic study of flocculation as a function of salt and salt kind, with and without dissolved gas, shows that the classical DLVO theory of colloid science is erroneous by some orders of magnitude. The results are in agreement with the theoretical predictions of Ninham. (*S. Wall [Dept. Physical Chemistry, Goteborg U., Sweden]; B.W. Ninham*)

Casimir Forces

The Casimir force has now been calculated analytically in the case of an intervening plasma at any temperature. The results have a bearing on the nature of black body radiation and the present controversy on direct measurement of forces between metal surfaces. They are also relevant to catalysis, metal adhesion and a number of practical problems. (J. Daicic [Institute for Surface Chemistry, YKI Stockholm]; B.W. Ninham)

Wetting Properties of Grafted Flexible and Semiflexible Polymers

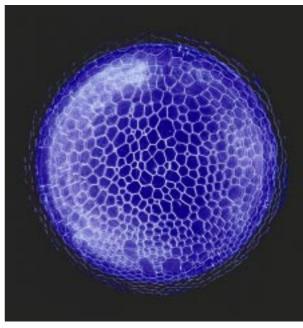
Polymers are often grafted to surfaces in the presence of a poor solvent. (The most notable example is air.) For the case of semi-flexible polymers we have shown that in a poor solvent the chains undergo a bending or tilting transition. For flexible polymers, we have shown that a uniform grafted layer is unstable to the formation of holes, thus forming a "holey layer". We have also shown that the surface can form "octopus surface micelles", where the chains bunch into groups. (J.N. Bright, D.R.M. Williams)

Surfactant Aggregate Shape and Topology

Our Guinier small-angle X-ray scattering apparatus (SAXS) is now in continuous use. We are looking at the possibility of detecting shape changes and topological defects in lypotropic mesophases induced by temperature and concentration changes, by tracking the variation of scattering peak position with those variables. Results are encouraging, though conclusions remain somewhat dependent on the assumed behaviour of the surfactant chains during dilution/heating. Systems studied include dihexadecyldimethylammonium bromide-tetradecane-water, novel steroidal surfactants in water, and proprietary novel surfactant mixtures being developed for cosmetic applications. (*S.T. Hyde, T. Sawkins; B. Folmer [Institute for Surface Chemistry YKI Stockholm]; M. Olla, S. Watanabe [KAO Corp]*)

Thin Diblock Copolymer Films on Striped Surfaces

Symmetrical diblock copolymers are made up of two covalently linked chemically immiscible blocks (of equal size) that are predicted to microphase separate in the melt into layers of one block, followed by another block etc. Growth of these melts on striped templates, promoting layering may reduce defect formation. The competition between the two length scales in the problem i.e., bulk layer spacing and size of the stripes, leads to some novel physics. So far we have shown in certain limits this problem maps onto the Frenkel-Kontorowa model of solid-



Soap bubbles formed between spherical surfaces exhibit strikingly different morphology from those commonly seen

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state physics, where aperiodic layer spacing develops. Numerical simulations of these systems have also been carried out to determine the validity of our analytical results. In another scenario, if the stripe width is much larger than the lamellar period, the substrate can induce a ridge-like surface topography. This is related to the formation of islands and holes in thin block copolymer melts. We investigate this problem and consider the possible grain boundaries in this system. (*G. Pereira, D.R.M. Williams*)

Thin Films of Rod-Coil Diblock Copolymer

Rod-coil block copolymers differ from their coil-coil counterparts by having one inflexible (or rigid) block connected to a flexible part. We have been investigating the thin film morphology of symmetrical rod-coil melts. These systems may form either smectic-A (untilted rods) or smectic-C (tilted rods) layers. The system is much more constrained than the coil-coil analog. (*G. Pereira*, *D.R.M. Williams*)

Mesoscale Physics

Biomineralisation in Sea Urchins

Work on the formation of ultrastructured magnesian calcite crystals in sea urchin shells continues. Novel proton tomography experiments (Physics, U. Melbourne) have yielded some useful structural data on the crystal morphology that we are processing, in an attempt to precisely map the topology and geometry of the calcite ultrastructure. (S.T. Hyde; F. Meldrum [Queen Mary and Westfield College, London]; A. Sakellariou [U. Melbourne])

Gel Crystallisation of Inorganic Carbonates

We have studied colloid aggregation of barium carbonate, crystallised in silica gels (pH 9-10), that forms curved sheet-like and "spiral" aggregates whose forms and dimensions mimic those of the earliest known fossils. Field emission scanning electron micrographs reveal the presence of very small prismatic single crystals aggregated with smoothly varying orientation within the aggregates, akin to the orientational order in molecular liquid crystals. The geometry of the spiral forms, from twisted ropes to croissant-like blobs, has been modelled by a single intersecting-surface – the twisted sphere. (*S.T. Hyde, N. Welham; J-M. Garcia-Ruiz [U. Granada]*)

Computation of Three Dimensional Crystalline Frameworks

We are in the process of deriving a catalogue of crystalline network topologies. Our approach is to construct graphs in the 2d hyperbolic plane (H²), and then embed those graphs in 3d Euclidean space (E³) by wrapping H² onto triply periodic hyperbolic surfaces. The hyperbolic nets are generated from decorations of arbitrary hyperbolic orbifolds. We have studied in some depth the generation of "thickets" in E³, that are multiply connected interwoven graphs, generated from closed-packings of trees in H², or hyperbolic "forests". These thickets offer



Close-up of a Sea Urchin Shell

interesting models for novel polycontinuous structures in block copolymers and molecular crystals. (S.T. Hyde, S. Ramsden; C. Oguey [Université Cergy-Pontoise])

Surfactant-Polymer Interactions in Structured Solutions

Using SAXS, small angle neutron scattering, neutron reflectivity, freeze-fracture electron microscopy and polarising optical microscopy we focus on the lamellar, hexagonal and cubic phase regions of surfactant/polymer/water mixtures. Our data on these systems reveals the polymer position within a liquid crystalline hydrophobic-hydrophilic matrix and provides evidence of the polymer-polymer interactions. (*E.Z. Radlinska*)

Lung Surfactants

The structure of the alveolar lining of lungs had been thought to be "tubular myelin", a lamellar-type phase. A more complex hyperbolic structure has been established. The results have obvious application to sudden infant death syndrome diagnosis and treatment, and for research into asthma and other medical conditions. (K. Larsson, [U. Lund & Malmo]; B.W. Ninham)

Microstructured Fluids and Templating of Nanoparticles

The microstructure of the aerosol Aersol-OT-water-isooctane phase diagram has been unravelled and yields to very simple geometric analysis. New concepts that have emerged – and are quite general properties of mesostructured fluids – are supra-aggregation, and interdigitised micelles. The results throw important light on the meaning of "phase", and allow nanoparticles of any size and shape to be tuned up at will. (*M-P. Pileni [Université P et M Curie Laboratoire, Paris]; B.W. Ninham*)

Modelling Fluid Flow in Natural and Model Porous Morphologies

(i) Oil Recovery from Rocks

We have continued with the development of a fast and efficient simulator for describing the flow of several immiscible fluids inside a porous material using the network model for two- and three- phase fluid flow. We can now simulate flow in networks of general topology, including those describing the medial axis of actual pore spaces in rocks, obtained from X-ray computer tomographic (CT) data. The software is now unique in its capacity to calculate and present visually the effects of pore space heterogeneity, network topology and three-phase drainage, all on networks with up to several hundred million nodes.

In collaboration with a group at SUNY at Stony Brook, we have made direct measurements of flow-relevant geometric properties of a number of sandstone samples. We have developed statistical models that mimic the geometric and topological properties and the spatial correlations, including correlated heterogeneity with different cut-off length scales. We are also investigating the effect of correlated heterogeneity on two-phase flow. The simulation results are consistent with the experimental data only if the heterogeneity of the pore space is correlated.

Our software is also being employed to investigate the role of topology in percolation processes, with the aim to use percolation as a characterisation tool. (A.P. Sheppard, R.M. Sok, T.J. Senden; W.V. Pinczewski [Petroleum Engineering, UNSW]; M.A. Knackstedt; W.B. Lindquist [SUNY Stony Brook]; M. Sahimi [U. Southern California])

(ii) Liquid Penetration into Timber Products and Paper: The role of pore morphology

Capillary imbibition of liquids into complex materials controls many industrially important processes, from ink printing (that relies on the removal of a pigment solvent) to gluing of timber products, including corrugated board and clay-coated paper. Network models of porous media provide a rich testing ground for relating pore-scale morphology and surface chemistry to bulk penetration behaviour. The mechanisms of droplet penetration into porous media are being investigated in a range of 2D micromodels. The theoretical model we have developed offers a microscopic description of different imbibition events at the pore scale, and the time scale of the events. From a description of the basic imbibition mechanisms one can model liquid penetration into complex two- and three-dimensional networks of pores. Concurrently, we are collecting data (in three dimensions) of the relevant network of a variety of papers using X-ray CT imaging. (M.A. Knackstedt, T.J. Senden; M.B. Lyne [International Paper])

Escape Transitions of Compressed Polymers

In many practical situations, most notably in biology and in colloidal science, a polymer chain will be compressed by a small obstacle. If this obstacle is not much bigger than the chain then an "escape transition" can occur, where part of the chain escapes from under the obstacle. We have recently undertaken two new investigations of this problem in order to clear up some controversy regarding the existence and nature of the escape transition. These studies presented exact statistical-mechanical solutions of the problem. (D.R.M. Williams; J. King, E.M. Sevick [RSC])

Bulk Chemical Physics

Semi-flexible Polymers in Poor Solvents

Semi-flexible polymers are different to their more usual flexible counterparts in that they have a significant degree of rigidity. Some biological examples are DNA and F-actin. When these polymers condense they form a toroidal rather than spherical structure. We have investigated the deformation of such a structure when adsorbed to a flat surface, when stretched between two points and under compression between flat plates. We determine phase diagrams and derive force laws for the system.

In order to place a 1 nanometre-long piece of DNA in the nucleus, the DNA must first be condensed using a protein. The collapsed DNA forms a number of novel morphologies, the most notable being the toroid. One major puzzle concerning these toroids has been the fact that they are all almost the same size, irrespective of the length of the DNA. We have explained this phenomenon, and have also predicted the existence of a new morphology — that of the hollow sphere. *(I.C.B. Miller, D.R.M. Williams, G. Pereira)*

Mixed Oxygen Electrolytes

Mixed oxygen electrolytes exhibit significant ionic and electronic conductivity. Such materials have potential applications in pressure-driven oxygen generators and partial oxidation reactors. The non-stoichiometric ferrite $\text{SrFeO}_{3-\delta}$ (0.0 $\leq \delta \leq$ 0.5) is an example of such a material that can be further chemically doped with alkali and transition metals and rare earths. A series of thermogravimetric and calorimetric experiments have enabled us to draw up a large part of a phase diagram and derive thermodynamic quantities that allow us to predict the composition of the oxide over a broad range of temperatures and oxygen partial pressures. The crystal structure was studied using conventional powder X-ray diffraction and high-resolution powder diffraction at the Australian National Beamline Facility in Tsukuba, Japan. A series of preliminary neutron scattering experiments (carried out with Professor S.J. Campbell of ADFA-UNSW) proved to be a very useful technique for investigation of structure and magnetic properties of the oxide. (M. Schmidt)

Cluster-assembled Carbon Nanofoam Produced by Ultra Fast Laser Ablation

A new fractal amorphous carbon nanofoam with a large fraction of tetrahedrally-bonded atoms was produced by high-repetitionrate laser ablation. Structural analysis of the foam has been performed with the help of Transmission Electron Microscopy, X-ray scattering, and electron energy-loss spectra. It has revealed that the foam is a novel fractal aggregate of near spherical clusters. The interior of such a cluster is a hyperbolic graphite sponge generically called "schwarzites". This form of carbon, which has an extremely low density and rather high surface area, is not only of particular academic interest, but also promises important applications such as, for example, hydrogen fuel cells, or containers for the lithium battery. (E. Gamaly; A.V. Rode, B. Luther-Davies [LPC]; S.T. Hyde; R.G. Elliman [EME]; A.S. Kheifets [AMPL/TP]; D.R. MacKenzie, S. Balcock [U. Sydney])

Formation of Single-wall Nanotubes with Continuous-Wave CO₂ Laser Ablation

We applied our kinetic theory of carbon nanotube formation in the gas phase to the analysis of experiments on nanotube formation at the Instituto de Carboquimica in Zaragoza, Spain. The influence of different experimental parameters on the structural features of the tubes formed has been elucidated. In particular, the theory predicts a simple dependence of nanotube length on the ambient gas pressure: the length is proportional to the mean free path of a single carbon in a carbon-gas mixture. (*E. Gamaly; A.V. Rode [LPC]; W. Maser; E. Mu-oz, A.M. Benito, M.T. Martinez, G.F. de la Fuente [Instituto de Carboquimica, Spain]*)

Instrumentation

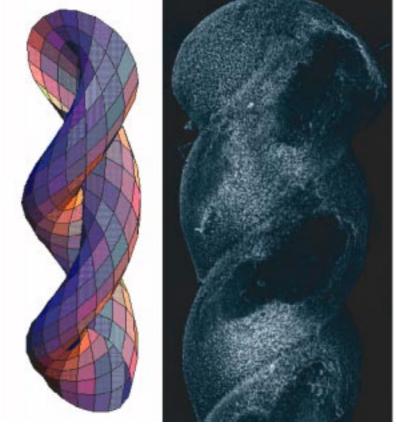
Capacitance Dilatometry in a Surface Force Apparatus

The forces between colloidal surfaces that in general may be opaque have been measured with a capacitance dilatometry attachment for the surface force apparatus. The method permits measurements of forces between opaque surfaces over periods of time ranging in suitable circumstances from tens of milliseconds to days. An equivalent circuit model for the electronic system has been developed that allows linear and

accurate measurement of displacement over a large fraction of the separation between the plates of the capacitor and which may have applications in other areas of transducer technology. (A.M. Stewart, T.J. Sawkins)

Friction Attachment

An attachment for the investigation of friction in surfaces of defined geometry in a surface force apparatus has been assembled. The frictional force is applied with a spring or magnet system, and frictional motion is detected by a strain gauge assembly. (A.M. Stewart, A.M. Hyde)



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Research Accomplishments



Professor Stephen Buckman - Head of Atomic & Molecular Physics Laboratories



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Atomic & Molecular Physics Laboratories

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.

Recent years have witnessed substantial changes in the staffing of the laboratories and also in the profile of our research activities. There have been marked successes in obtaining external funding for new and exciting initiatives that are now coming on line. These include the ultracold, metastable helium atom trap, the condensed matter (e,2e) spectrometer and the photodetachment/photofragmentation spectrometer. In addition, throughout this year there have been new experimental activities commencing in electron scattering from molecular radicals (the subject of a joint RIEF grant with Flinders University) and new UV laser sources (a joint RIEF grant with Macquarie University), as well as theoretical support for the atmospheric modelling work in the form of an ARC Large Grant (held jointly with the University of Adelaide). We were also successful in obtaining an ARC International Fellowship (Professor Hyuck Cho) for work in Electron Physics. Also, towards the end of the year, the UV Physics Unit was successful in securing one of the five IAS Fellowships which were offered as a result of the most recent round of strategic initiative funding. This was an extremely competitive process and is an indicator of the strength of both the research proposal and the successful candidate.

However, whilst the Department has shown that it is capable of generating new and exciting ideas which can attract external support, the main challenge that we face in the immediate future is how to staff these activities. We have maintained academic staff numbers via ARC and other fellowships but the continuing success of our research activities is critically dependent on graduate students and, unfortunately, their numbers continue to slowly decline. The Department presently has less than half the graduate student cohort that we boasted five or six years ago and the effects of this are starting to be felt on the research effort. We remain committed to providing a first rate environment for our graduate students and this year several students (Dean Alle, Jenny Gibson, Dragana Milic, Phillip Palma, James Sullivan) graduated.

Once again there have been many personal achievements and recognition gained by members of the Department during 1999. Emeritus Professor Robert Crompton was awarded the Order of Australia in recognition of his outstanding services to science and society; Dr Anatoli Kheifets was awarded a Fellowship by the Science and Technology Agency of Japan to conduct collaborative research in Japan for two months; Dr Julian Lower spent a month in Germany as a guest of the University of Freiburg; Professor Stephen Buckman was awarded a Fellowship by the Japan Society for the Promotion of Science for a one month visit to Japan.

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

Low-energy Electron Scattering and Spectroscopy

Low-energy electron collision studies remain at the heart of the activities of the Electron Physics Group. As in previous years these studies have involved the measurement of absolute electron scattering cross sections, the spectroscopy and dynamics of transient negative ion states formed in electron collisions and the development of new experimental techniques for the study of these processes.

Absolute cross section measurements have continued with the study of elastic scattering from both nitrous oxide (N₂O) and benzene (C_6H_6). The N₂O experiments have been conducted as part of a collaboration with Professor Tanaka's group at Sophia University in Tokyo. The main aims were to cross-check results for absolute cross sections from two quite different electron spectrometers and to combine results for elastic scattering and vibrational excitation measured on the two different apparatus. This project has also acted as a catalyst for an ongoing collaborative effort between the two groups. (*J.C. Gibson, R.J. Gulley; H. Tanaka [Sophia U., Japan]; S.J. Buckman*)

The benzene measurements represent the further extension of our measurements to studies of large molecules. Benzene is the simplest of the stable aromatic hydrocarbons and represents a large molecule that is tractable for theoretical calculations. An extensive set of absolute elastic scattering cross sections have been compiled and are being prepared for publication. These results have also provided further insight into the structure of several low-energy negative ion resonance states that manifest themselves strongly in the scattering cross sections. (H. Cho [Chungnam National U., Korea]; R.J. Gulley, L.J. Uhlmann; S.J. Buckman)

In recent years our systematic studies of low energy elastic scattering from diatomic and polyatomic molecules have revealed an interesting, and apparently ubiquitous, structure at forward scattering angles and low energies (3-7 eV) in the differential scattering cross section. The similarities in this structure (a shoulder or minimum/secondary maximum in the cross section) between the many systems we have studied is quite striking and the process responsible for its formation apparently pays little heed to molecular structure, polarizability or dipole moment. We are approaching this effect as a likely manifestation of classic rainbow (multiple) scattering from the (aligned) atomic constituents of the molecule. The corresponding critical rainbow



The new electron momentum spectrometer

scattering angles θ_c must be determined by molecular structure and dimensions, and work continues on the development of an analytical explanation. (*L.T. Chadderton, S.J. Buckman*)

Studies of transient negative ions (resonances) formed in electron scattering from metal vapours have continued this year. Measurements in cadmium were completed and analysed and a new set of experiments on magnesium has commenced. In order to obtain a complete picture of the resonance structure in Group II atoms, it is proposed that the next target will be mercury. (J.P. Sullivan, R. Panajatovic, D.S. Newman, S.J. Buckman)

Construction and assembly of the recoil atom spectrometer, which is to be used on the metastable atom beam line, (see Atom Manipulation Project) has continued. It is hoped that this apparatus will be ready for testing early in 2000 and attached to the beam line later in the same year (*L.J. Uhlmann, R.J. Gulley, S.J. Buckman*)

A set of electron scattering cross sections for molecules is being prepared for a new edition of the Landolt-Bornstein Tables. (*M.T. Elford; M.J. Brunger [Flinders U.]; S.J. Buckman*)

Electron Momentum Spectroscopy of Solids

The construction of the new, high-energy electron momentum spectrometer has been completed and the first measurements have been performed. These reveal good count rates and resolution in combination with a low background due to multiple scattering. This has led to a significant improvement of the energy-resolved momentum densities that can be obtained with this spectrometer. The sample preparation facility was extended to include ion sputtering and ion etching. The spectrometer is easy to use and seems to operate with remarkable reliability. New insight into the electronic structure of different forms of carbon has already been obtained and the measured energy-momentum distribution of electrons in the valence band of carbon resembles those of the many-body calculation quite well. The calculation is based on the novel technique utilizing the cumulant expansion to the one-electron Green's function in the realistic crystalline environment (see Theoretical Physics section for detail).

More solid state targets will be investigated next year, both experimentally and theoretically. These measurements should be able to validate our theoretical approach to the many-electron correlation in solids. (*M. Vos, A.S. Kheifets, E. Weigold*)

Atoms, Molecules, Radiation, and the Nanoworld

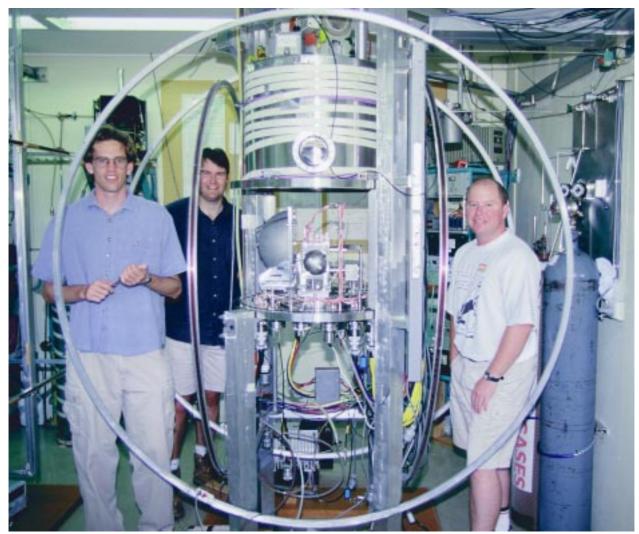
At the heart of this group of projects is a planned progressive extension of the Department's overall research coverage in at least three specific ways. First, we are investigating the interaction of radiation with matter at far higher energies (for example 4.5 GeV heavy uranium ions with crystals). Secondly, we are studying the fundamental act in nanomolecular self assembly of the 'new' and in general larger nanostructures, including for example the fullerene C_{60} molecular family, and corresponding nanotubes. Finally, we are carrying out a variety of experiments using various electron microscopic techniques directed at three-dimensional nano quantum dot arrays on superlattices in crystals.

For the interaction of general ionizing radiation (electrons, Xand γ -rays, GeV ions, MeV C₆₀ cluster projectiles etc.) in what will be a long study, we have started to lay down an atomic selection rule theory for macroscopic crystal target 'response' based on the explicit bonding properties of the atomic constituents. It has been conclusively shown, for example, by both experiment and theory that Bragg's rule of additivity for compound stopping powers generally does *not* apply, being grossly violated by detailed and material specific atomistic (point defect) energy absorbing processes. Similarly the ability of an energetic single atom or cluster ion to register as a particle "track" is entirely dependent on detailed target response. Track models based on instantaneous energy deposition from projectile to lattice therefore fail and, because of specific recovery processes, measured track widths are in general meaningless.

The new 40 MeV C_{60} cluster ions continue to prove themselves the most remarkable of atomic projectiles, barely studied as yet. The huge effective charge gives them a huge energy deposition density, and there is "steric electronic stopping" – a completely new phenomenon due to the first 'half' of the molecular projectile creating a 'plasma' through which the second half must pass (nonlinear stopping power). In certain solids C_{60} cluster ions can generate long, regularly intermittent tracks demarked by sharp polyhedral metallic colloid clusters each no more than 6-7 nm in size. The detailed electronic properties of these quantum dot arrays are under investigation. New work on the formation of carbon and boron nitride nanotubes (with J.S. Williams and Chen Ying [EME]) has been extended and generalized. It has been shown that ball-milling of a powder progenitor produces seed material rich in homogenous and/or heterogeneous nucleation sites for nanotube growth during subsequent controlled anneal. Nanotube growth is due to surface self-diffusion of atomic species and is more readily controlled than other current methods, such as in laser ablation or arc discharges of graphite. (*L.T. Chadderton*)

Atom Manipulation Project

Experiments using the metastable helium, magneto-optic trap (MOT) were the focus of work in the Atom Manipulation Project this year. The trap is loaded using metastable helium atoms produced by the bright beam machine (which was also used for experiments on conducting atoms through hollow optical fibres – see Laser Physics Centre report). The MOT has been improved to confine in excess of ten million atoms in a cloud, approximately 4 mm in diameter, at temperatures below one milliKelvin. A new trap density diagnostic (based on the differential phase shift between two phase modulation side bands on a probe laser) was developed in our collaboration with the Atom Optics group in the Department of Physics, The Faculties, and now enables sensitive, non-destructive measurement of changes in the trap density.



Andrew Daley (Vac Scholar), Dr Robert Gulley and Stephen Battisson by one of the Department's crossed beam spectrometers

Theory of Atomic Double Ionization Atomic double photoionization 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 ionization has been a spectacular success. Angular correlation and energy sharing between the two photoelectrons as well as the circular dichroism in helium double photoionization were predicted by the CCC model with high accuracy, and

as well as the circular dichroism in helium double photoionization 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 photoionization from closed-shell atomic targets such as noble gas atoms. (*A.S. Kheifets; I. Bray [Flinders U.]; A. Ipatov [St. Petersburg Technical U.])* **Inverse Scattering Theory** This year, we continued the development of a new technique for phase-shift analysis in multi-channel scattering. This technique

phase-shift analysis in multi-channel scattering. This technique makes use of the unitarity condition on the scattering matrix. By solving coupled nonlinear equations, the complete scattering matrix can be extracted from the experimental differential cross section. The technique will be applied initially to electron scattering. The scattering energy will be chosen such that only the ground state and the first excited state are open channels. (*A. Purwanto, D.R. Lun, R.P. McEachran, S.J. Buckman*)

Atomic Scattering Theory

There have been several calculations of elastic electron scattering from heavy atoms based on the Dirac equations. However, these calculations have included only the lowest-order interelectron interaction, the Coulomb interaction. In a recent calculation for elastic scattering from Xe and Hg, the next lowest two-body term, the frequency independent Breit interaction has been added. Although the effect of including this term on the differential cross section was minimal, small changes were found in the parameters that describe the spin polarization of the scattered electron. (*A. Demise [York U.]; R.P. McEachran; J.W. Darewych, A.D. Stauffer [York U.]*)

The relativistic distorted-wave method has been used to study the electron impact excitation of the heavy noble gases Ar, Kr and Xe. Results for spin polarization parameters, electron-photon coherence parameters, as well as differential cross sections were determined and compared with previous semi-relativistic calculations and experiment. Overall good agreement with experimental measurements of the differential cross section and the coherence parameters were obtained. Notably different results for spin polarization parameters are predicted compared with previous semi-relativistic calculations. (*R.P. McEachran; A.D. Stauffer [York U.]; R. Srivastava [Roorkee U.]*)

Positron Interactions with Atoms

The elastic cross sections for positron scattering from both Ar and Kr have been determined by the polarized-orbital method while the corresponding excitation and ionization cross sections have been determined within a distorted-wave framework in an

The improved MOT and its diagnostics were employed in a series of novel experiments on electron scattering from the excited (2^3S_1) state helium atoms. An electron gun producing a high flux, pulsed electron beam is used to scatter electrons from the trap contents. The total scattering cross section is determined by monitoring the trap loss rate and the electron beam current density, that is measured using a combination of crossed wires and a Faraday cup. Preliminary measurements show promising results, which should improve upon existing total cross section measurements that have inherently large uncertainties.

The trap has also been used for initial studies of sub-recoil cooling of trapped metastable helium atoms using velocity selective coherent population trapping (VSCPT). This technique employs two counterpropagating and oppositely circularly polarised laser beams to create two superposition states of the degenerate magnetic sublevels of the $2^{3}S_{1}$ state. Cooling below the photon recoil temperature can occur as the atoms randomly walk into the "dark" superposition states following successive interactions with the laser, after which they remain at zero velocity because the "dark" state no longer interacts with the light field. The two dark states are also separated in momentum by two units of the photon recoil velocity, which results in an "atomic beamsplitter" since the atomic centre-of-mass wavefunction is separated into two partial waves (the superposition states). Work is continuing on this experiment, which will use light tuned to both the 1083 nm trapping transition and 389 nm radiation produced by an improved frequency doubled Ti:Sapphire laser, to create well separated coherent wavepackets with applications to atom interferometry. (M.D. Hoogerland, M. Colla, R.G. Dall, R.J. Gulley, L.A.W. Robinson, J. Swansson, L.J. Uhlmann, S.J. Buckman; K.G.H. Baldwin [LPC])

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

This research focuses on uncovering the reaction mechanisms underlying electron-atom scattering processes through the performance of highly specific collision experiments. The main focus of this research is the investigation of the process of electron-impact ionization, its dependence on the kinematics of the reaction and upon target structure. By using beams of spin polarized electrons and spin polarized and oriented atoms, we are able to focus on, and individually highlight, the effects of electron exchange and spin orbit coupling acting on bound and free electrons, target orientation and the effects of electron correlation in the final state.

This year significant refinements in our measurements on laserexcited, spin-polarized sodium atoms have been achieved. Working closely with our theoretical colleagues our latest results reveal the conditions under which exchange scattering plays a significant role in the break-up process and provide insight into the way angular momentum transfer from the target the final electron pair affects the result of experiment. Such measurements present a severe test to scattering theory and thereby significantly contribute to further progress being made in this direction.

Development is continuing on the technical front in the development of a new generation electron spectrometer which is anticipated to yield three to four orders of magnitude improvement in data collection capabilities, and enable the measurement of subtle effects beyond the capability of existing devices. (J.C.A. Lower, E. Weigold)

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energy range up to 200 eV. The relative contributions of these individual cross sections to the total cross section were analyzed and compared to recent experimental measurements. The overall agreement with experiment is quite satisfactory except in the threshold region. (*R.P. McEachran; L.A. Parcell [Macquarie U.]; R.I. Campeanu [Seneca College, Toronto]; A.D. Stauffer [York U.])*

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

Positron Binding to Atoms

The investigations into the existence and structure of positronic atoms continued to provide unique insights into the behaviour of positrons with atoms and molecules.

An investigation into positron binding to a model alkali atom (based on sodium) provided a great deal of information about the nature of the positronic atom bound state. One notable feature of this research was the realisation that there is a competing attraction between the positron and residual ion core to attract the valence electron that has a major impact upon the structure of the positronic atom. In addition, the results of the model calculations showed why positron binding was possible in lithium and sodium, but not possible for potassium, rubidium and cesium. A calculation of positron binding to atomic zinc was successfully carried out with the Fixed Core Stochastic Variational Method (SVM). This calculation was very intensive and consumed a year of computer time. Even then, it is likely that the positron binding energy of 0.039 eV could easily be uncertain (too low) by as much as a factor of two.

This technique was also used to establish that positronium could bind to potassium. It was also demonstrated that the structure of HPs, LiPs, NaPs and KPs could be thought of as a positronium atom loosely bound to the parent atom. The LiPs, NaPs and KPs systems all had annihilation rates within 5% of the (spinaveraged) annihilation rate of the Ps ground state. This result and plots of the electron-positron correlation function

demonstrated that these systems could be roughly described as Ps bound to the neutral atom. The calculation for KPs was also very expensive and took almost a year to complete.

The widely used Configuration Interaction (CI) method was applied to the problem of positron-atom binding. Although the CI basis is not the best basis with which to investigate positron binding, the initial series of calculations indicated that the method could be used to predict positron binding in a modest time, and also predict the positron binding energy to an accuracy of about 10%. The first CI calculation performed was on positronic copper (e+Cu) and was able to verify an earlier prediction of positron binding made with

the fixed core SVM. A later test calculation upon positronium hydride (PsH) obtained 85% of the binding energy. In addition, pilot calculations on copper positride (CuPs) and positronic cadmium (e⁺Cd) gave strong evidence (predictions were rigorous with respect to the underlying fixed core Hamiltonians) of positron binding.

The stability of some exotic atoms with two positrons was established. Following communications from Dr K. Varga (Argonne National Laboratory, USA), it was established that the positronium molecule (Ps_2) could be bound to the lithium and sodium cations. Analysis of the electron-positron correlation functions was used to establish that the structures could be best described as a Ps_2 molecule orbiting the Li⁺ and Na⁺ ion cores. (*J. Mitroy, G. Ryzhikh, M.J. Bromley*)

Experimental Detection of Positronic Atoms

Our calculations indicate that the positron affinity for copper (and silver) is less than the electron affinity. This makes the experimental measurement of the positron affinity a possibility. We have therefore proposed an experimental protocol where a Cu^- beam is scattered with a positron beam and Cu^+ ions downstream of the interaction region are measured. Neglecting collisions of Cu^- ions with the background gas, the only reaction that can produce Cu^+ ions for centre-of-mass collision energies less than 1.8 eV involves the prior formation of e^+Cu . Besides verifying the stability of positronic copper, the experimental protocol could be applied to other atoms (such as tin) which are promising candidates to bind a positron. (*J. Mitroy, G. Ryzhikh*)

The Dynamics of Positron Annihilation

A detailed investigation was carried out of the electron-positron annihilation process in the light systems PsH and e⁺He(³S^e). This was a pilot investigation setting the ground work for more extensive studies of the annihilation process in larger systems and ultimately the condensed matter phase. This also provided the foundation for a study of electron-positron annihilation during positron-hydrogen collisions.

The insight gained from our investigation of bound states was used to render an existing explanation of the electron-positron



The new photofragment spectrometer takes shape

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Computational Techniques for Atomic Structure Calculations

Of essential importance to our research has been the use of the orthogonal pseudo-potential (OPP) to represent the electrons in the core of bigger atoms. The first detailed computational investigation of the behaviour of the OPP was presented for publication.

A Hartree-Fock program written and used extensively by the author has been published. This program should be useful to other researchers in atomic physics. (J. Mitroy, G. Ryzhikh)

Diffusion of Meteor Trails

The study of the diffusion of electrons in meteor trails that commenced in 1997 has continued during 1999. 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 [U. Adelaide]; R. Robson [James Cook U.])

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 highresolution laser-spectroscopic techniques.

Measurements are continuing of collision-induced features in the spectrum of molecular oxygen, in the energy range of the 3pRydberg states. The previously unseen ${}^{3}\Delta_{\mu}$ state has been identified and indications of interesting quantum-interference effects unearthed. (B.R. Lewis, S.T. Gibson, E.H. Roberts)

While experimental work in high-resolution VUV laser spectroscopy has been limited during the year by construction of the Photofragment Spectrometer and significant laser failures, work has continued on the measurement of cross sections in the Schumann-Runge system of O2 near the first dissociation limit at 175 nm. Analysis of these spectra, which are complicated by many perturbations, is continuing, some significant progress having been made on this challenging problem. (K. Waring, B.R. Lewis, S.T. Gibson; K.G.H. Baldwin [LPC])

The measurements just discussed were performed using narrowbandwidth coherent radiation generated by the four-wave difference-frequency mixing of high-power dye-laser radiation in a nonlinear medium (Xe). The best resolution routinely available using this technique in the VUV is ~0.1 cm⁻¹ full-width at half-maximum. We have recently embarked on a collaborative project with Professor Brian Orr, Macquarie University, to develop an injection-seeded solid-state laser system that is intended to yield a significantly increased resolving power in such VUV studies. Following a successful RIEF proposal for 1999, we have recently acquired the YAG pump laser for this project. In addition, a successful ARC Large-Grant proposal for 2000 will help to facilitate the development of this new highresolution source that should significantly enhance our spectroscopic capabilities. (K.G.H. Baldwin [LPC]; B.R. Lewis; B.J. Orr [Macquarie U.])

Resonance-enhanced Multiphoton Ionization (REMPI)

Our analysis of the (2+1)-photon REMPI spectra of the 3s Rydberg states of O2 has been completed. The results of this collaborative study have shown that the analyzed spectra are of rather poor quality, and have led to the measurement of new, better-calibrated spectra in several international laboratories. By the application of our coupled-channel Schrödinger-equation technique to the interpretation of the strong Rydberg-valence perturbations in these spectra, we hope to gain a definitive insight into the molecular structure of O_2 in this energy region. (B.R. Lewis, S.T. Gibson; R.A. Copeland [SRI International, California]; M.L. Ginter [U. Maryland]; J.S. Morrill [Naval Research Lab, Washington DC])

New measurements on the (3+1)-photon REMPI spectra of O₂ in the region of the 3p Rydberg states have been completed. The results show a number of very interesting, pressure-dependent, quantum-interference effects which are in the process of interpretation. We now believe that, contrary to our initial interpretation in terms of intracollisional interference, 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]; R.A. Copeland [SRI International, California])

Photofragmentation

Construction of the MEC-funded Coincidence Photodetachment/ Photofragment Spectrometer is progressing. 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 beamline of this instrument has been established and the crucial ability to isolate anions of a specific mass has been verified. The photodetachment stage will be completed with the installation of a time-of-flight photoelectron detector. A successful RIEF proposal in 1999 has led to the acquisition of a YAG pump laser, the final piece of apparatus necessary to enable operation of the spectrometer in photofragment mode. (S.T. Gibson, E.H. Roberts, B.R. Lewis, S.J. Buckman; K.G.H. Baldwin [LPC])

Atmospheric Computation

Work has continued on an ARC-funded project involving quantum-mechanical modelling of the transmission of solar VUV radiation through the Earth's atmosphere. This study has incidentally resulted in the discovery of a new sum rule involving the lineshape asymmetry in cases of weak molecular predissociation by optically-inactive continua. The main aim of this project remains to provide a comprehensive database to be used extensively by the community of atmospheric geophysicists in their photochemical models. In this respect, it is encouraging that our initial reports of this work have led to an invitation to present the research at the XXV Symposium of the European Geophysical Society in 2000.

The atmospheric transmission calculations will be tested against new high-resolution cross-section measurements performed in our VUV laser-spectroscopy laboratories. These new measurements will be facilitated by the award of an IAS Fellowship which hopefully, will be taken up in 2000. (B.R. Lewis, S.T. Gibson; L.W. Torop, F.T. Hawes [U. Adelaide])

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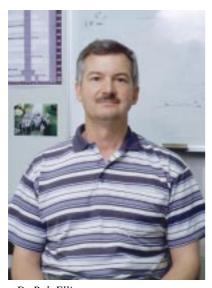
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Research Accomplishments



Dr Rob Elliman - Head of Electronic Materials Engineering



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

Electronic Materials Engineering

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 covers a full spectrum, from fundamental to applied projects, and can be broadly classified into four pursuits: Ion-Beam Modification and Analysis of Materials, MOCVD Growth of III-V Semiconductors, Electronic and Optoelectronic Devices, and Materials Characterization.

Department staff and students published in excess of 122 papers in peer-reviewed journals and domestic and international conferences, including seven invited or keynote presentations — an outstanding performance. Additional cross-collaborative publications not included above are included in Section 5. Much of the research was collaborative, with more than 75% involving co-authors external to the ANU. More than 25 scientists/students (national and overseas) visited the School to use EME's facilities as part of such collaborations. Staff also made major contributions to the administration of the School, the University, and professional societies, and served on the editorial boards of several key international journals, as highlighted in latter sections of this report. The Department's contribution in the key fields of semiconductor processing and ion beam analysis was also recognised by the international community, with international conferences in each of these areas to be chaired by EME staff within the next two years. In addition, an international workshop on semiconductor optoelectronics was held in the School in March.

In terms of staff achievements, the highlight of the year was the promotion of Dr C. Jagadish to full Professor, a well-deserved promotion. Our students were also very successful again this year. Three students were awarded PhD degrees in 1999 and all received outstanding referee reports from national and international reviewers. The Department's Founder's Day presentation was given by C. Lobo, and A. Dowd represented the Department in the competition for the John Carver Prize. Four new students commenced their PhD studies in the Department this year, one of whom – T. Weijers (joint Honours and PhD student with Nuclear Physics) – was awarded a University Medal for her Honours project undertaken in the Department. The Department also hosted one Honours student and two undergraduate project students.

External income continued to be an essential ingredient for the success of the Department and several new opportunities have emerged this year. One of the most exciting opportunities was the announcement by a major Taiwanese semiconductor manufacturer (LEDEX) of their intention to establish a development laboratory, "BlueLab" in Canberra. The proposed investment is around \$US11M and it is anticipated that the laboratory will contain a suite of facilities for growth and processing of GaN and related materials. The international reputation of EME's optoelectronic devices program and the unique cluster of growth, processing and characterization facilities were major reasons for this decision. Indeed, LEDEX has already established R&D links with EME – two engineers from LEDEX visited EME for three months in 1999 – and the company intends to apply for a major "START" grant (jointly with EME) in early 2000. Another significant industry interaction involved a research contract (\$0.5M over two years) with Aixtron, the supplier of the new MOCVD reactor, to be installed early in 2000. This contract involves the growth and characterization of a number of indium phosphide-based structures with applications in advanced fibre communications. In addition, the semiconductor device achievements in EME, such as the specifications of the high power 980 nm laser, have generated significant international interest and a grant has recently been obtained from the Department of Industry, Science and Resources (DISR) to develop a business model for commercialising semiconductor devices in Australia. Other significant R&D contracts with the Australian company AMBRI for

biosensors, and with DSTO for infrared photodetectors are also currently in progress. The Department was also very successful in competing for funds and was awarded an ARC postdoctoral fellowship (jointly with NP), an international research fellowship, DIST Bilateral Science and Technology Grants, an international collaborative program grant with Sweden, ANTSO grants for access to major international facilities, an Australia-Korea Foundation Grant, as well as the research contracts outlined above. The Department also participated in ARC Large Grants (or RIEF grants) to be held at the Universities of Canberra, Melbourne, New South Wales, Wollongong and Newcastle.

The unique array of research equipment and facilities housed in the Department continues to be one of its strengths. This year, funding of more than \$1.8M was received for two new major facilities, an MOCVD reactor and an ion-accelerator for ion beam analysis. The existing MOCVD laboratory is being modified to accommodate the new reactor and a new laboratory has been constructed for the accelerator. The reliability and utility of our existing facilities, and the installation and development of new facilities, depends heavily on the professionalism, skill and dedication of EME's technical staff (T. Halstead, M. Aggett, A. Hayes, A. Watt, B. King, D. Llewellyn) and externally funded technical assistants (M. Conway, A. Williams). EME's departmental administrator, L. Walmsley has also made an outstanding contribution to the smooth running of the department. The Department also acknowledges the contribution made by School administrative and technical staff, including those in the electronic and mechanical workshops, and plumbing and joinery shops.

MOCVD Growth and Device Fabrication in III-V Semiconductors

Both the MOCVD growth and optoelectronic device activities are led by Professor C. Jagadish. One of the highlights of research during this year was the growth of indium phosphide based quantum-well structures particularly with lattice matched InGaAs and InGaAsP layers. A new research program which involves the deposition of self assembled monolayers of organic molecules on semiconductor surfaces was initiated in collaboration with CSIRO, and brings together biomimetic engineering and semiconductor physics. Studies on quantum dots have shown interesting and distinctly different carrier transfer mechanisms in high-density and low-density dot structures. In the area of devices, reactive ion etching studies of GaN epitaxial layers under various plasma conditions led to etch rates as high as 130 nm/ min. Quantum well intermixing of quantum well infrared detectors has produced large shifts in detection wavelength enabling the fabrication of two-colour detectors. Photodetectors operating at 1.55 µm were successfully grown as part of a defence contract. The fabrication of the highest power (1.8 Watt) quantum well laser operating at 980 nm, in collaboration with colleagues at Eindhoven University of Technology, was one of major highlights of research in the device area. Vertical cavity surface emitting lasers were also fabricated using novel processing techniques developed in the Department. All these areas involved extensive collaboration (for example, with seven other Australian universities and more than 10 overseas laboratories). Progress in specific research projects is outlined below.

Lattice matched epitaxial structures based on InP/InGaAs and InP/InGaAsP grown by MOCVD have shown excellent electrical and optical properties. This material system is of particular



Christine Carmody and Dr Hoe Tan loading the MOCVD reactor

significance as it allows access to the optical communications wavelengths of $1.3 \,\mu\text{m}$ and $1.55 \,\mu\text{m}$. Quantum well intermixing studies were initiated using both SiO₂-induced and ion implantation-induced interdiffusion. Large energy shifts were observed without any degradation in optical properties of the structures. (*H.H. Tan, C. Carmody*)

In the area of quantum dots (QDs), the photoluminescence (PL) temperature dependence of high density QD samples (Arrhenius behaviour) is attributed to carrier thermal emission and recapturing into neighbouring QDs. Conversely, in low density QD samples non-Arrhenius behaviour is observed, and thermal transfer of carriers between neighbouring QDs plays no significant role. Furthermore, the efficiency of carrier transfer into isolated dots is found to be limited by the rate of carrier transport in the InGaAs wetting layer. (*C. Lobo*)

The properties of dielectric layers of SiO_x and Si_xN_y deposited by the new Plasma Enhanced Chemical Vapour Deposition (PECVD) reactor have been studied. Process parameters were found to significantly influence the composition, porosity, and H content of the layers. For example, the porosity was found to increase with decreasing deposition temperature whereas oxide composition and deposition rate were found to be dependent on nitrous oxide flow. (*P.N.K. Deenapanray, L. Fu, H.H. Tan, K. Gaff [OSC]*)

Quantum-Well-Intermixing studies on GaAs/AlGaAs and InGaAs/AlGaAs structures were carried out using SiO_x , Si_xN_y cap layers. For the first time, a correlation between the dielectric layer properties and interdiffusion in quantum well structures was found. In particular, porosity in the deposited layers was found to enhance the interdiffusion in quantum wells, leading to enhanced PL energy shifts. Time-resolved PL measurements have shown that the carrier transfer is much faster in interdiffused quantum wells, which has been attributed to changes in the composition gradients introduced by the impurity-free interdiffusion process. (*P.N.K. Deenapanray, L. Fu, H.H. Tan*)

In the area of 980 nm high power lasers, work in collaboration with Eindhoven University of Technology, resulted in a record output power of 1.8 Watts. These lasers are widely used in optical communication systems as pump sources for optical amplifiers. Novel designs, based on low optical confinement along with optical trap layers, and novel growth processing led to this record output power. Further efforts are underway to improve power output by the creation of non-absorbing mirrors using selective area interdiffusion. Dual wavelength lasers were successfully developed using novel MOCVD growth techniques. These structures required the growth of current-blocking layers and etching, followed by a subsequent growth of active regions. (*H.H. Tan, L. Fu, M. Buda; G. Iordache, G.A. Acket, T. van de Roer, F. Karouta [Eindhoven UT]*)

Research on quantum well infrared photodetectors (QWIPs) was very fruitful, leading to the fabrication of two-colour QWIPs. Multiple energy implantation produced excellent intermixing results, leading to a clear shift in the detector photocurrent spectral response. Interestingly, bound-to-quasi-bound as-grown QWIPs changed into bound-to-bound QWIPs after interdiffusion, leading to a narrowing of spectral response. (*L. Fu, N. Li, H.H. Tan*)

Research on vertical-cavity-surface-emitting-lasers (VCSELs) continued with further improvements in the processing techniques. Thermal oxidation of high Al-containing AlGaAs layers was optimised, and enhanced interdiffusion of quantum wells below the oxide layers during subsequent thermal processing was observed. For certain Al thicknesses interdiffusion was suppressed, whereas thick Al layers led to further enhancement in PL energy shifts, suggesting enhanced interdiffusion. Modelling of these results is underway. VCSELs were fabricated using an oxide for electrical confinement giving excellent threshold and light emission characteristics. (*M.I. Cohen, H.H. Tan; A.A. Allerman [Sandia National Labs]*)

In collaboration with colleagues from the University of Canberra, a wide variety of semiconductor lasers were fabricated with the goal of achieving low noise lasers. To achieve this goal, it is necessary to obtain high internal and external quantum efficiency and low-threshold current densities. The requirement to undertake the noise measurement at low temperature necessitated the development of suitable mounting techniques. This was successfully achieved and mounted devices are currently under investigation. (J. Hazel, L. Fu, H.H. Tan, A. Uddin, P.J. Edwards, W. Cheung; G. French, R. Gill, G. Kumar [U. Canberra])

In a joint effort with the Laser Physics Centre and the Optical Sciences Centre, semiconductor saturable absorber modulators were developed. These were grown by MOCVD and subsequently irradiated with high-energy ions to achieve subpicosecond carrier lifetimes. Transmission electron microscopy (TEM) in conjunction with optical characterization provided an understanding of the role of defects in controlling the modulation characteristics of these saturable absorbers. (*M.J. Lederer, B. Luther-Davies [LPC]; N. Akhmediev [OSC]; H.H. Tan, C. Jagadish*)

Ion Beam Modification and Analysis of Materials

The Ion Beam Modification and Analysis of Materials Group is led by Dr R.G. Elliman and employs world class facilities, including three ion-accelerators, to undertake and support a wide range of research projects ranging from fundamental studies of radiation effects in materials to the fabrication of electronic and optoelectronic devices. It also supports a broad range of national and international collaborations involving for example CSIRO, ANSTO and five state universities in Australia and more than 10 overseas laboratories. Research highlights have been quite diverse. Of particular note is the ongoing collaboration with the Nuclear Physics Department in the area of high-energy, heavyion beam analysis of materials. This work has received considerable national and international attention, with three invited talks presented at international conferences on a new detector and its applications. Other highlights have involved an understanding of irradiation-induced defect evolution in Si, insitu Transmission Electron Microscopy (TEM) observations of defect interactions with, and shrinking of, cavities in Si, production and study of properties of implantation-induced nanoparticles in SiO₂, non-equilibrium processes associated with metal gettering in Si, understanding of compound formation (oxide and nitride layers) in Si during SIMS, major insights into ion and photon-induced desorption processes and local bonding arrangements in ion-irradiated semiconductors. With regard to major facilities, the most significant development this year was the purchase of a new ion-accelerator to replace the ageing Van

Research School of Physical Sciences & Engineering 1999

de Graaff accelerator currently used for ion beam analysis. The new accelerator will extend existing capabilities by providing higher-energy beams. Research progress in projects involving ion-beam modification and analysis are summarised below. The ion beam analysis work includes research using the Riber secondary ion mass spectrometry (SIMS) apparatus led by Dr M. Petravic.

Ion Beam Modification of Materials

The potential causes of defective recrystallisation in amorphised III-V semiconductors continued to be investigated. In particular, the influence of macroscopic non-stoichiometry on the solid-phase epitaxial growth (SPEG) of amorphised GaAs has been studied with TEM. This technique has also been utilised to image the excess Ga precipitate depth distributions to identify constituent element diffusion during the annealing process. (*K.B. Belay, D.J. Llewellyn, M.C. Ridgway*)

Extended X-ray absorption fine structure (EXAFS) studies of a variety of amorphised semiconductors have yielded the first atomic-scale structural parameter measurements for such materials. Experiments were performed at both the Photon Factory, Japan and the Stanford Synchrotron Radiation Laboratory, USA. The coordination number of Ga and As atoms in amorphous GaAs decreased whilst the opposite was apparent for In atoms in amorphous InP. The presence of chemical disorder (In-In bonding) was verified for amorphous InP. The structural evolution of irradiated Ge, prior to the onset of porosity, was attributed to the production and retention of defective configurations within the amorphous phase. Such changes were only apparent through the use of advanced EXAFS analysis. (*C.J. Glover, M.C. Ridgway, G.J. Foran [ANSTO]; K.M. Yu [Lawrence Berkeley National Lab]; A. Nylandsted Larsen [Aarhus U.]*)

In collaboration with the Department of Nuclear Physics and the University of Bonn, perturbed angular correlation (PAC) was utilised to characterise In probe-point defect complexes in ionimplanted Ge. Two distinct probe environments have been observed to date. (*C.J. Glover, M.C. Ridgway, A.P. Byrne [NP]; R. Vianden [U. Bonn]*)

Further progress has been achieved in the understanding of the implantation-induced phenomena resulting from ion irradiation of silica as appropriate for optical waveguide formation. Loss measurements, as a function of ion mass, dose, energy and annealing temperature, have been performed. Thereafter, chemical etching in combination with atomic-force microscopy was utilised to measure changes in implantation-induced density and refractive index as functions of depth. (*C.M. Johnson, M.C. Ridgway, T.D. Thompson; V. Gurarie [U. Melbourne]*)

In a new initiative, synthesis of long wavelength N-containing III-V semiconductors was achieved using N implantation. Recently, N was found to decrease the band gap of III-V semiconductors grown by MOCVD. N implantations were carried into GaAs, AlGaAs, InGaAs, InP to achieve up to 5% N. PL studies have shown emissions at long wavelength, suggesting reduction in the band gap of these materials, as confirmed by photoreflectance studies. (*H.H. Tan, C. Jagadish*)

Ion implantation studies have been initiated to study amorphisation processes in InP and InGaAs-based epitaxial structures. Custom structures of InP and InGaAs layers were grown by MOCVD and irradiated with both keV and MeV ions. Initial Rutherford Back Scattering (RBS) and channelling measurements are providing interesting insights into disordering/ reordering processes in these materials. (*H.H. Tan, C. Jagadish*)

Deep level transient spectroscopy (DLTS) and TEM studies have been carried out to study defect evolution in ion irradiated and annealed n-type Si and p-type Si. Below the threshold dose for extended defect formation, DLTS revealed no point defect signatures in n-type Si, whereas, point defects were observed in p-type Si. Under majority carrier injection, DLTS could detect only vacancy-related levels in n-type Si but both vacancy and interstitial-related levels in p-type Si. These results suggest that residual defects are interstitial in nature in n-type Si, hence their absence under majority carrier injection. From TEM, extended defects were found to be rod like {311} defects for Si implantation and both {311} defects and {111} loops were found in Ge and Sn implanted and annealed samples above the threshold dose. TEM characterization of {111} loops suggested they were formed from amorphous pockets during Ge and Sn implantation. (J. Wong-Leung, S. Fatima, J. Fitz Gerald [RSES]; C. Jagadish)

Significant advances were made in the understanding of the nonlinear optical response of Ge-implanted silica. In particular, the magnitude and temporal response of the nonlinearity were shown to be similar for samples implanted at 77K and room temperature, and in samples annealed to 1000°C. TEM confirmed the presence of nanocrystals in samples irradiated at room temperature and those annealed to 1000°C but showed no evidence for crystallites in samples as-implanted at 77K. This suggests, for the first time, that the nonlinear response does not depend on the presence of nanocrystalline Ge. Studies are underway to elucidate the role of Ge. The PL intensity from silicon nanocrystals embedded in silica was shown to increase with increasing nanocrystal concentration up to a critical value and to decrease for higher concentrations. It has been speculated that the reduction in intensity at high concentrations is due nanocrystal-nanocrystal interactions that transfer energy from the radiative to non-radiative fraction of crystallites. Hydrogen passivation of the nanocrystals, which enhances the emission intensity by more than an order of magnitude, was also shown to produce an irreversible red-shift in the PL emission, consistent with H induced growth of the nanocrystals during the lowtemperature passivation treatment. (A. Dowd, S. Cheylan, R.G. Elliman; M. Samoc, B. Luther-Davies, N. Manson [LPC])

A new project commenced on the fabrication of a Si nanocrystalenhanced optical amplifier. This project is based on the fact that the PL emission from Er-doped silica can be increased by more than an order of magnitude in the presence of Si nanocrystals. Preliminary modelling has shown that the increase in refractive index caused by the Si nanocrystals acts to confine the optical modes to the active region of the waveguide. This should further increase the gain of the amplifier. (*R.G. Elliman, A. Ankiewicz* [OSC]; B. Stritzker)

Charge transport was investigated in metal-insulatorsemiconductor (MIS) structures that were ion-implanted and annealed to produce Si crystallites in the insulating SiO_2 layer. Shifts in current-voltage and capacitance-voltage curves were observed after the application of a forward-biased voltage stress or exposure to ultra-violet (UV) light. Negative photoconductivity (i.e. the conductivity reduces by exposure to UV light) was also observed for the first time. These effects were explained by photoionisation and charging of Si nanocrystals and charge transport in the SiO₂ film. PL and electron-spin resonance (ESR) were also used to study intrinsic defects in fused silica during ion-implantation and annealing procedures designed to form H-passivated Si nanocrystals. Ion implantation reduced the PL emission from 288 and 390 nm diamagnetic oxygen-deficient defects and produced nonradiative paramagnetic defects, as measured by ESR. (*S-H. Choi; J. Martin [LPC], S. Cheylan, R.G. Elliman*)

In a collaborative project involving the CNRS in Paris and the University of Melbourne, crystalline Si containing a band of nanocavities has been irradiated with Si at various temperatures to study the interaction of defects with cavities. A range of interesting phenomena were studied by in-situ and ex-situ TEM and ion channelling. At and slightly above room temperature, the cavities are observed to be preferential nucleation sites for amorphisation of Si under ion irradiation. The explanation for this behaviour is that the cavities can provide free volume for local expansion of Si necessary to form less dense amorphous Si. At an irradiation temperature of 300°C, where amorphous layers are not formed, cavities are efficient sinks for Si interstitials, thus giving rise to a zone around cavities that is denuded of residual defects. It is also found that cavities shrink and disappear at higher irradiation doses either via plastic flow of amorphous Si into cavities, or at higher temperatures, via the accumulation of excess Si interstitials at cavities. (X.F. Zhu, M.C. Ridgway; J.C. McCallum [Melbourne U.]; J.S. Williams, M.C. Conway; F. Fortuna, H. Bernas [CNRS])

Two aspects of ion beam induced epitaxial crystallisation (IBIEC) have been examined with an attempt to understand the process in more detail. Specifically, the dependence of IBIEC on ion mass and energy deposition density has shown the process does not scale exactly with the number of displaced atoms at the interface as the energy density is increased. This implies that defect interactions at an amorphous-crystalline interface can inhibit crystallisation. Further experiments involving IBIEC under channelling conditions for both buried and surface amorphous layers have clearly indicated the crucial role of

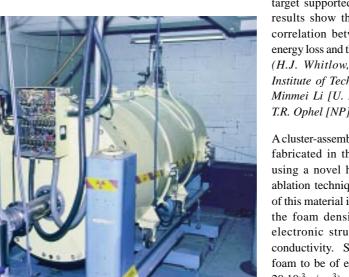
cascade effects (ie, interface displacements from Si recoils) in IBIEC. To date all results strongly support irradiation-induced atomic displacements within a few atom layers of the interface as the major determinant of IBIEC. (*J.S. Williams, M.J Conway, I. Young; A. Kinomura [ONRI]*)

Studies of ion implantation damage in GaN have accelerated in 1999 with the availability of good quality material from LEDEX in Taiwan and a new PhD project. Detailed studies have been undertaken on damage build-up under irradiation with several ions. Preferential surface disordering is observed in all cases, even at liquid nitrogen irradiation temperatures. This process is associated with surface trapping of mobile defects but leads to severe dissociation and loss of nitrogen at higher doses. (S.O. Kucheyev, J.S. Williams, C. Jagadish, G. Li [LEDEX]; S.J. Pearton [Florida])

Materials Preparation, Analysis and Characterisation

Work has continued on the development and application of the heavy-ion elastic recoil detection (HI-ERD) system. This technique, which employs high-energy heavy ions, such as 210 MeV ¹⁹⁷Au, provides quantitative compositional analysis of the material, including low atomic number elements such as H. This collaborative project between EME and Nuclear Physics has led to the development of an advanced position-sensitive gasionisation detector, incorporating several novel design features to simplify data collection and analysis. These include a modified electrode structure to reduce distortion of the electrostatic field used to collect electrons and the incorporation of a second grid electrode for measurement of the total ion energy. (*H. Timmers, T.R. Ophel [NP]; T. Weijers, S. Jones, R.G. Elliman*)

The correlation between energy loss and collected charge for individual ions traversing 7.1 μ m self-supporting Si p-i-n Δ E detectors has been studied using the Enge spectrometer in the Nuclear Physics Department. In this work the simultaneous measurements of the Δ E signal and energy loss were made for 49 MeV ²⁸Si and 103 MeV ²⁸Si and 147 MeV ⁷⁴Ge incident ions obtained by 10° scattering of a primary beam from a thin gold



End of an era, after 37 years service, the Van de Graaff accelerator is about to be replaced

target supported on a carbon foil. The results show that there exists a strong correlation between the individual ion energy loss and the collected charge signal. (H.J. Whitlow, Yanwen Zhang [Lund Institute of Technology], D.J. O'Connor, Minmei Li [U. Newcastle], H. Timmers, T.R. Ophel [NP], R.G. Elliman)

A cluster-assembled carbon nanofoam was fabricated in the Laser Physics Centre using a novel high-repetition-rate laser ablation technique. The characterisation of this material included measurements of the foam density, its surface area, its electronic structure and its electrical conductivity. Such analysis showed the foam to be of extremely low density (2- $20 \cdot 10^{-3}$ g/cm³) with its surface area in the range 300–400 m²/g. The measured high sp³-bonding fraction at the edges of the foam, and at the edges of the cluster, are a clear indication in favour of the proposal



Jody Bradby loading samples into the microhardness tester

based on high resistivity of the foam, that the sp³-bonding atoms are located mostly at the surface of the clusters, and that the connections between the clusters are due to sp³-bondings. (A.V. Rode; E.G. Gamaly, S.T. Hyde [AM]; R.G. Elliman, N. Welham; B. Luther-Davies [LPC]; D.R. McKenzie, S. Bulcock [U. Sydney])

The use of reactive oxygen and nitrogen ions in SIMS analysis constitutes an interesting area for investigation of fundamental ion-induced near-surface chemical reactions. The different segregation behaviour of impurities during oxygen bombardment of Si (under conditions favouring formation of thin surface oxides) has been studied for a number of ion implanted metals. We have demonstrated, for the first time, the antisegregation of F into the oxide as an electric field builds up across the surface oxide during ion bombardment. Further, we have shown that the electric field plays the dominant role in segregation of Li and K out of the oxide and have identified the thermodynamic component of the segregation driving force. We have also explained the controversial segregation behaviour of Ca reported in the literature by taking into account two components of driving force for segregation: the electric field and the larger solid solubility of Ca in amorphous Si than in Si oxide. (P.N.K. Deenapanray, M. Petravic)

Within the angular interval favouring formation of surface compounds under reactive ion bombardment, we have identified several different types of angular dependence for the broadening of SIMS profiles. For the first time we have shown that a range of impurities in Si, such as Ga, B, Ge and Sb, exhibit a dramatic degradation in depth resolution around a "magic" impact angle of 27° from the surface normal. We have explained this behaviour by enhanced surface roughening (confirmed by atomic force microscopy) around the critical angle for surface oxide formation. Nitrogen bombardment does not show any such dramatic change in angular dependence due to the extremely low mobilities of different impurities in silicon nitride. However, observed small changes in depth resolution have been found to closely follow the changes in silicon nitride stoichiometry. (*M. Petravic, P.N.K. Deenapanray, C.M.Demanet, D.W. Moon*)

Research into the mechanisms and applications of the gettering of metals to cavities in Si continued apace. This study involves international collaboration with researchers in Japan and USA and has employed a number of characterisation methods including neutron activation analysis (NAA), RBS/ion channelling, TEM and SIMS. A major thrust has been in understanding the non-equilibrium (defect-mediated) processes that lead to super-efficient accumulation of metals at cavities and the pathways (and bottlenecks) to thermal equilibrium during thermal annealing. (J.S. Williams, J. Wong-Leung, M. Petravic, M.J. Conway, B. Stritzker; A. Kinomura [ONRI]; D.J. Eaglesham [Lucent])

Studies began in 1999 (in collaboration with USA scientists) to assess the stability of metal trapping to open volume defects in Si. Two types of open volume defects are being studied, namely nanometre sized cavities and vacancy clusters, the latter being associated with so-called $R_p/2$ defects obtained after energetic ion irradiation, particularly at room temperature and above. Results indicate that oxygen (if present in the wafer) can result in ejection of metals from the walls of open volume defects and loss of efficient gettering for metals during annealing. For Au, it is observed that the number of Au atoms trapped in open volume defects scales with the magnitude of the open volume. Interesting trapping and release phenomena have been observed when different types of defects (at different depths) are present in the Si. SIMS has been the major analysis technique but TEM and RBS/channelling have also been used. (J.S. Williams, M.J. Conway, J. Wong-Leung, M. Petravic, P.N.K. Deenapanray; R.A. Brown [NJIT]; D.J. Eaglesham [Lucent])

A new student project began in 1999 involving nanoindentation of a range of semiconductor structures using EME's UMIS machine. To date the indentation load/unload curves have been measured for crystalline and amorphous Si and the residual indentations studied by AFM and Scanning Electron Microscopy (SEM). (J. Bradby, J.S. Williams; M.V. Swain (U. Sydney])

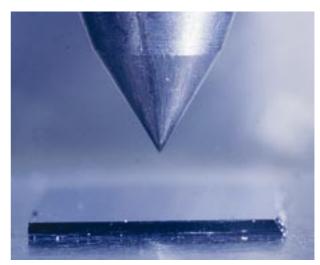
Photoemission and photodesorption of positive hydrogen ions from hydrogenated GaAs surfaces has been studied using synchrotron radiation in collaboration with colleagues in France (Synchrotron Research Facility in Orsay). It was shown, for the first time in a covalent system, that a striking similarity exists between the shape of ion-desorption curves and corresponding photoelectron spectra around core-level binding energies of As and Ga. This correspondence suggests that the excitation of core electrons in As and Ga atoms plays a dominant role in the desorption of H⁺. A new method has been introduced in order to determine the contribution from different desorption channels. We have shown that a comparison of desorption yields from hydrogenated surfaces of different termination (polar and nonpolar surfaces) can provide evidence for a particular desorption channel (a direct process in our case). Further, by tuning synchrotron radiation to a particular energy, hydrogen atoms bonded to a specific site may be selectively removed from the surface. (M. Petravic, P.N.K. Deenapanray; G. Comtet, L. Hellner, G. Dujardin, B.F. Usher [U. Paris-Sud])

DLTS studies on low dose ion implanted p-Si examined the generation rate of point defects as a function of ion mass. The generation rate of the divacancy was found to deviate from a linear dependence for high-mass ions, particularly Sn. In order to understand this behaviour, high temperature Sn implants were carried out, giving an increase in divacancy concentration for a fixed dose. This suggests that suppression of amorphous pockets at high temperatures may lead to changes in divacancy concentration. (*S. Fatima, C. Jagadish, B.G. Svensson*)

A fundamentally new solid-state process has been developed for the formation of C and BN nanotubes. This synthesis method involves two separate steps: a cold mechanical milling followed by a relatively low temperature (< 1400°C) thermal anneal. Ball milling of both graphite and crystalline BN compound first produces nanosized particles or clusters with a microporous structure. After annealing, the material has reordered, predominantly to the hexagonal crystal form in both C and BN and varying yields of hollow nanotubes have also been observed. These range in diameter from 100 nm (for the BN – complex segmented tubes) down to 5 nm (for C – probably single-walled nanotubes). The most interesting observation is that nanotube growth of C and BN appears to occur at relatively low temperatures by a solid state process rather than via vapour phase or liquid phase transport. (Y. Chen; L.T. Chadderton [AMPL], J.S. Williams, M.J. Conway, M. Bruckard; J. Fitz Gerald [RSES])

Titanium diboride can be made by ball milling for between 10 and 15h, with the valuable high purity powder obtained by selectively leaching the unwanted residue. The same synthesis route can be used to make a large range of transition metal carbide, nitride and boride phases that are much sought after as industrial materials in cutting tools and high temperature materials. The final particle size is invariably sub-micron and crystallographic studies indicate that they are single crystal, making them ideal for manufacturing purposes. A second area of investigation has been the enhanced dissolution of minerals after extended milling. Recent work has shown that a tantalum/ niobium ore undergoes a dramatic dissolution rate increase following milling. (*N. Welham*)

The relationship between crystal structure and stoichiometry (oxygen content) is an important issue for mixed oxides such as strontium-iron oxide, which is a material used for oxygen conductors (sensors) and fuel cells. Thermal analysis, X-ray diffraction (also at elevated temperature) and neutron diffraction have been used to provide new understanding for such material systems for compound powders prepared by ball milling. (*M. Schmidt*)



The microscopic diamond tip of the microhardness tester

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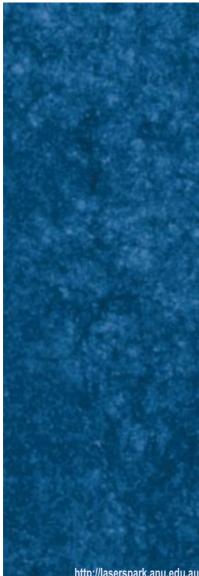


Research School of Physical Sciences & Engineering 1999

Research Accomplishments



Professor Barry Luther-Davies - Head of Laser Physics Centre



Laser Physics Centre

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

Research Summary

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. A collaboration involving Professor Luther-Davies and Dr Krolikowski, with members of the Optical Sciences Centre, resulted in a successful application to the University's Performance and Planning Fund (PPF) for work on Nonlinear Science and Solitons. Outside the School we have projects with the Departments of Chemistry and Physics and Theoretical Physics at the ANU; ADFA; James Cook University; University of Sydney; and overseas groups in USA, Germany, UK, Poland, France, Switzerland and Russia.

The Centre remains a significant contributor to the expanded Australian Photonics Cooperative Research Centre which was funded by the Government for a further seven year period early in the year. Professor Luther-Davies was reappointed as Research Director for the CRC and as one of the Directors of Australian Photonics Pty Ltd that is the Commercial and Management agent for the CRC. The CRC is expected to fund expansion of the Department's work on novel photonic materials and devices including an ongoing commercially sponsored project on fibre optic voltage sensors (FOVS).

Two new staff members joined the Centre during the year. In June Dr Max Lederer took up an ARC funded SPIRT Post Doctoral Fellowship, supported by Electro Optic Systems Pty Ltd, and Dr Robbie Charters took up a SPIRT funded PDF, with support from AOFR Pty Ltd. Therese Martin joined the FOVS project as a part-time research assistant, and Daniela Werner joined the Centre from the FH Aalen University of Applied Sciences, Germany, to undertake practical training also on the FOVS project. A cohort of PhD students, some with historical links to the Centre, completed their PhDs. They included Doug Body, Jason Christou, Hugo Giordano, Max Lederer, Wenqian Yu, Geoff Pryde, Bruce Stenlake and Weijian Lu. A further significant personal achievement was Anita Smith's selection to represent the ANU at the 8th International Women in Leadership Conference at Edith Cowan University in November.

We were pleased to welcome a number of visitors during the year. Professor Byeong-Soo Bae from KAIST Korea is spending twelve months in the Centre supported by an IREX grant to work on silica-zirconia sol-gel glasses. Dr Abdolnassar Zakery from Shiraz University in Iran joined the Centre in October to work on pulsed laser deposition of chalcogenide glasses. Alex Boiko from Electro Optic Systems Pty Ltd continues to produce high quality optical coatings in support of the research as well as servicing the needs of the company. Dr Yanjie Wang and Dr Yue Gao, also from Electro Optic Systems remain as long term visitors. Short-term overseas visitors included Professor Eric Van Stryland from CREOL at the University of Central Florida, Dr Christian Bosshard from ETH Zurich, and Dr Nick Zheludev from the University of Southampton, UK. Dr Graham Atkins from the Optical Fibre Technology Centre at the University of Sydney is a regular visitor working on organically modified silicate (ORMOSIL) materials for photonics.

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

Nonlinear Optical Materials and Structures

We continue to study the nonlinear optical properties of materials for applications in photonics as well as developing models of substances important for the understanding of the microscopic origin of nonlinear optical effects. In addition to the classes of materials studied previously, of particular interest this year has been the nonlinear properties of gallium-silica interfaces, and the behaviour of polyenes with different chain length.

Third-order NLO Properties of Conjugated Polymers and Model Molecules

We have established that some π -conjugated polymers have large but complex third-order nonlinear optical properties. Examples of such materials are poly(indenofluorene) which exhibits very strong absorption saturation for femtosecond laser pulses at 800 nm, and polymers of the poly(phenylenevinylene) family, which exhibit both very strong self-focussing and/or self-defocussing effects and nonlinear absorption. In collaboration with overseas groups we have investigated several polymers and π -conjugated molecules with the aim of finding materials with both the optimized nonlinear properties and good processability to be useable for low loss planar waveguide structures. While several polymers offer promise as good materials for nonlinear waveguides with low loss nonlinear merit factors, the real part of the electronic third-order susceptibilities are not among the highest measured at 800 nm. Finding a good compromise between factors such as the low optical loss and high nonlinearity at a useful operating wavelength, as well as good environmental stability, remains a challenge in this field. Both the fundamental and technological aspects of this research will be immensely enriched next year with the acquisition of a tunable source of high-power mid-IR femtosecond pulses with the aid of a RIEF grant. (A. Samoc, M. Samoc, B. Luther-Davies)

Nonlinear Properties of Organometallic Compounds

We have continued investigations of NLO properties of organometallic compounds in collaboration with the group of Dr M.G. Humphrey of the Chemistry Department in the Faculty of Science. A highlight of this year's research has been the



Doped optical fibre fluoresces under UV light

determination of nonlinear optical properties of a family of organometallic dendrimers: compounds with finely crafted spatial structures and with very strong nonlinear absorption properties. The effects of substitution and the resulting changes of the multipolar electronic structure on the nonlinear optical properties have been studied. (*M. Samoc, B. Luther-Davies, M.G. Humphrey [Chemistry, The Faculties]*)

Development of Plastic Optical Fibres for Voltage Sensing Applications

We have been involved via the Australian Photonics CRC in a project sponsored by ABB and Transgrid to make plastic optical fibres as distributed voltage sensors for the power industry. The fibres rely on a novel mechanical alignment process acting on a specific structure of an electro-optic molecule in the fibre to create a sensitivity to voltage. The work this year was centred on obtaining single-mode optical fibres from a polymethacrylate material containing a specially designed electro-optically-active polymeric dopant in the fibre core. This research involved a diverse range of topics, from quantum mechanical calculations, through chemical synthesis in the two-stage preparation of fibre preforms, drawing of plastic fibres and to measurements of linear and nonlinear optical properties of the fabricated materials, and of optical fibres made from them. (B. Luther-Davies, A. Samoc, M. Samoc, R.M. Krolikowska, C. McLeod, T. Martin, J. Bottega, I. McRae)

Nonlinear Optical Effects at Gallium/silica Interface

The reflectivity of a gallium-silica interface held close to, but below, the gallium melting point of 29.8°C can be changed significantly (> 40%) by light over a very broad spectral range 400–1600 nm. The effect has been attributed to a surface-assisted phase transition from the stable α -gallium phase to a phase of metallic nature. We have investigated the nonlinear switching phenomena occurring at the interface between a thin film of gallium and a silica substrate. In collaboration with Dr N. Zheludev of the University of Southampton we are studying these effects on samples obtained at the Laser Physics Centre using pulsed laser ablation. The preliminary results indicate that gallium mirrors can show relatively fast (2 picosecond risetime and nanosecond relaxation time) switching for short laser pulses. (*B. Luther-Davies, A.V. Rode, M. Samoc, N. Zheludev [U. Southampton]*)

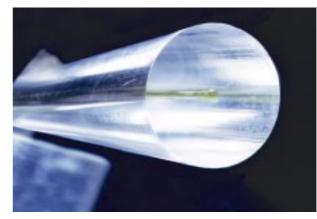
Semiconductor Nonlinear Optics and Applications

We have demonstrated for the first time that ion-implantation can be used to generate semiconductor optical materials with ultra-fast response $(10^{-13}-10^{-12}s)$ and well-preserved absorption modulation. The outcome of the study can serve as a guideline for ion-implantation in GaAs devices for applications such as ultra-fast all-optical switching and laser mode-locking using semiconductor saturable absorber mirrors (SESAMs). Work has begun to investigate beryllium or zinc doping of ion-implanted GaAs as a promising method to further increase the nonlinear modulation of implanted GaAs devices. We are also currently working on device design (SESAMs, all-optical switches and wavelength converters) incorporating quantum well structures of InGaAs/InP and other compounds suitable to extend passive modulator applications towards the communications wavelengths (i.e. 1.3 μ m and 1.55 μ m). The work involves collaboration with both the Department of Electronic Materials Engineering and ETH Zurich. (M. Lederer, B. Luther-Davies; H. Tan, C. Jagadish [EME]; M. Haiml, U. Siegner, U. Keller [ETH Zurich])

A picosecond SESAM mode-locked Nd:YVO₄ laser has been developed which provides variable output pulse duration through a simple and user friendly "on-the-fly" adjustment. A very low repetition rate (7MHz), SESAM mode-locked high power diode pumped laser is currently under development for use in ultra-fast laser ablation experiments. We have also continued with the design of an oscillator-amplifier combination for the picosecond satellite laser ranging systems for Electro Optic Systems Pty Ltd. A novel and efficient thermal management scheme for diode side-pumped high power lasers and amplifiers has been developed. Incorporated in a laser amplifier the scheme was shown to result in superior thermal management especially for laser crystals with poor thermal conductivity and strong pump absorption such as Nd:YVO₄. (M. Lederer, V. Kolev, B. Luther-Davies)

Photonic Materials and Devices

We have continued to work on 2×2 thermo-optic space switches created by the laser writing of single mode channel waveguide devices in a photosensitized form of poly-methylmethacrylate (PMMA). In particular, we have concentrated on a new class of switching device, the mode evolution or digital directional coupler (DDC), in which adiabatic refractive index tapers are created along the guide length, by continuously varying the laser scanning speed in a smooth, precise manner. Since the writing system is under direct software control, a large range of taper functions is accessible, resulting in high-performance mode evolution couplers with crosstalk levels better than -30 dB. Working from this optimized passive device design, it has been demonstrated that complete switching can be achieved in digital directional couplers through the thermo-optic effect. Since the



Close-up of the end of a fibre blank prior to drawing, clearly showing the yellow doped core

device operating principle is based on the adiabatic evolution of a single local normal mode along the device length, DDCs display such desirable characteristics as wavelength independent and polarization insensitive operation. These features make them well suited to wavelength division multiplexed telecommunications systems.

In collaboration with researchers from the Centre of Electronics and Microelectronics, University of Montpellier, an Organically Modified Silicate (ORMOSIL) exhibiting low loss at telecommunications wavelengths and a much-improved thermal stability compared to PMMA has been investigated. The laser writing process has been equally successful in this material system, resulting in the demonstration of many types of guided wave devices. In particular, multimode interference (MMI) splitter-based arrayed waveguide gratings with a wavelength selectivity of 2.0 nm have been routinely produced, and devices exhibiting 0.8 nm selectivity are under development.



Members of the photonic materials group

Research School of Physical Sciences & Engineering 1999

Work on new waveguide materials is proceeding through collaboration with Professor Byeong-Soo Bae from KAIST in Korea to develop photosensitive silica-zirconia ORMOSILs suitable for use with our laser direct write technology. In addition, collaboration with Dr Graham Atkins, University of Sydney, several new photosensitive sol-gel material systems have been developed. Preliminary investigations of laser written waveguides formed in these films have given excellent results. (*R. Charters, A. Samoc, M. Samoc, B. Luther-Davies; G. Atkins [U. Sydney]; B. Bae, O. Park [KAIST, Korea]*)

Soliton Physics

Experiments on spatial solitons in photorefractive media are carried out within the Laser Physics Centre, whilst theoretical analyses of the observed phenomena involve close collaboration with members of the Optical Sciences Centre. This year the major interest has been in a new class of partially coherent spatial solitons that can have variable shape. These exist in media with Kerr-like response when a beam consisting of a superposition of mutually incoherent beams is present in the medium. These solitons undergo shape transformation during collisions. The phenomenon has been observed experimentally in photorefractive media that, although deviating from Kerr-like behaviour, can mimic the Kerr response at least for short propagation distances. (W. Krolikowski; N. Akmediev, A. Ankiewicz A. Snyder [OSC])

Pulsed Laser Deposition of Novel Materials

We continue to develop our patented ultra-fast pulsed laser deposition (UFPLD) process for the creation of new materials including high quality thin films. We have upgraded our laser facilities to better approach the optimum for UFPLD. The upgraded laser generates trains of 25 - 35 laser pulses of 60 ps

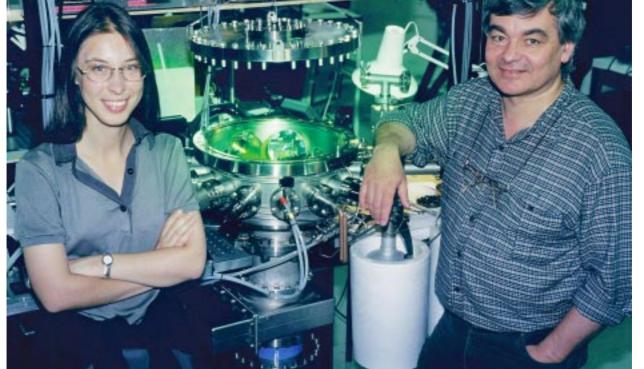
pulse width, at repetition rates from 2 to 20 kHz. Up to 45 W average power was available after amplification providing up to 5×10^{11} W/cm² on the target surface. Conversion of the laser beam into second harmonic (532 nm) light has allowed us to use UFPLD with a variety of dielectric materials with high absorption at this laser frequency. (*A.V. Rode, B. Luther-Davies*)

Cluster-assembled Carbon Nanofoam

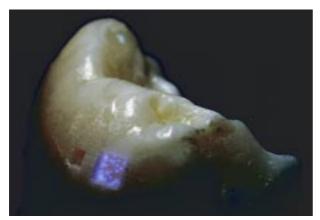
A new fractal amorphous carbon nanofoam with a large fraction of tetrahedrally-bonded atoms was produced by UFPLD. The efficient evaporation of carbon, which is beyond reach with other evaporation methods, resulted in a diffusion-limited aggregation of carbon atoms into clusters. The resistivity, measured in a collaboration with Dr R. Elliman EME, of $(1-3) \times 10^9$ Ohm·cm at room temperature and $(1-10) \times 10^{11}$ Ohm·cm at 80 K, is comparable with the RF-sputtered amorphous diamond-like carbon (DLC) film, while the density of the carbon foam is about 2 orders of magnitude lower than that of DLC. The currentvoltage (I-V) characteristics of the foam at various temperatures from 85–130 K are nonlinear and demonstrate a voltagedependent resistivity. The differential resistivity is approximately 10 times higher in the low-voltage region (<±30 V) than in the high voltage region (~±100 V).

Structural analysis of the foam performed using Transmission Electron Microscopy, X-ray scattering (in collaboration with Professor S. Hyde, AM) and electron energy-loss (in collaboration with Professor D. MacKenzie, University of Sydney) revealed that the foam has the following peculiar features that have not been observed before:

• The ablated carbon clusters which are ~6 nm in diameter, have a novel structure with well-defined structural units with a characteristic length of 5.6 ± 0.4 Å. The data indicate that the



Bronwen Taylor and Dr Andrei Rodé with the high power laser ablation equipment



The pulsed laser group continue to investigate a variety of new applications of femtosecond laser pulses, shown here: laser dentistry, note the accurately milled square in the human tooth and the purple plumes of plasma from the laser hits

structure is likely to be a graphite polymorph, generically called "schwarzites", which can be accomplished by warping of graphitic carbon sheets onto a random, isotropic hyperbolic sheet.

- In the larger micron-length scale the cluster-assembled carbon foam demonstrates a fractal ordering with the estimated fractal dimension of 2.4.
- The measured high sp³-fraction at the edges of the foam and at the edges of the clusters are a clear indication in favour of the proposal, based on high resistivity of the foam, that the sp³bonding atoms are located mostly at the surface of the clusters, and that the connections between the clusters are due to sp³bondings.

All these unusual features of this novel form of carbon, together with an extremely low density of 2–20 mg/cm³ and rather high surface area of 300–400 m²/g, are not only of particular academic interest, but also promise important applications, such as hydrogen supercapacitors. (*A.V. Rode; E.G. Gamaly, S.T. Hyde* [*AM*]; *B. Luther-Davies; R.G. Elliman [EME]; A.S. Kheifets* [*AMPL*]; *D.R. MacKenzie and S. Balcock [U. Sydney]*)

Acceleration of Ions in the Skin-effect Laser-target Interaction Regime

Ionisation of the laser-ablated vapours with lasers producing ns and ps duration pulses at various wavelengths has been studied in order to understand the mechanisms of the vapour-plasma transition. It has been established that there are several regimes characterising the laser-target interaction that depend on laser intensity, wavelength, and pulse duration. The range of laser intensities for optimal laser evaporation is determined by the condition of transparent vapours. The intensity range is upperlimited by the opaque plasma formation due to vapour optical breakdown.

The results are illustrated on laser evaporation of graphite with Nd:YAG laser (1.064 μ m), KrF laser (248 nm) and ArF laser (193 nm). For the UV-laser wavelength the regime of skin-effect interaction was proposed as the mechanism of ion acceleration, and the range of validity of the skin-effect mode was established. For UV lasers the interaction has a bi-modal nature: the interaction may proceed initially in the skin-effect regime

resulting in a few high-energy ions, until the hydrodynamic expansion begins at the later stage. The skin-effect interaction at the initial stage of the UV laser pulse gives, to our knowledge, the first explanation for acceleration of ions up to ~100 eV at low laser intensities of 10^8 - 10^9 W/cm², and ns-range pulse duration. (E.G. Gamaly [AM]; A.V. Rode, B. Luther-Davies)

Formation of Single-wall Nanotubes by High-repetition-rate and Continuous-wave Laser Ablation

We performed a theoretical analysis of the continuous wave CO₂ laser and the high-repetition-rate Nd:YAG vaporization processes that leads to the formation of single-wall nanotubes (SWNTs). After a simulation of the experimental details we model the absorption mechanism, evaporation rate, collision rates, scanning rates, and then focus on the gas and heat diffusion processes. With these basic considerations we can qualitatively explain the experimental results under static and dynamic conditions, including the influence of the buffer gas, and the gas pressure on the formation of SWNTs. We also found that the heat transport, kinetic and diffusion processes explain seemingly different formation conditions in qualitative and semi-quantitative agreement with the experimental results. A self-consistent scenario for nanotube formation in the gas phase has been identified and suggests future experiments for checking the formation mechanism. (E.G. Gamaly [AM]; A.V. Rode)

Solid State Laser Spectroscopy

There are two major research efforts within the Solid State Laser Spectroscopy Group. One is directed towards optical processing and computing. This is an experimental project involving a novel laser facility developed by the Group, which comprises a special laser with very good frequency stability. New measurements achieved during the year include demonstration of time domain optical processing and the first demonstration of multi-pulse NMR techniques in the all-optical regime. The second research area involves studying nonlinear absorption of multiple electromagnetic fields by quantum systems. All measurements performed this year involved a particular colour centre in diamond that has proven to be a model system. The optical pumping cycle in the colour centre is not well understood, but significant progress in quantitative fitting of spectra has been made this year in phenomenological modelling of the optical spin polarization process. The most spectacular use of the diamond centre, however, continues to be the observation of many fundamental nonlinear quantum optics effects that have not previously been seen experimentally.

Optical Computing and Processing

Many optical transitions of rare earth ions in solids have long dephasing times of the order of milliseconds and may be of value for coherent optical processing. With this in mind, over a period of many years we have developed a special optical system, including a laser with a stability at least matching the transition line width, and optical phase sensitive detection. With these two attributes we now have capabilities beyond that of any other laboratory working in this area.

The rare earth materials used are known to have potential as optical storage media. Optical pulses occurring within the dephasing time coherently interfere, and as a consequence the pulse sequence is stored in the material via spectral holeburning as a long-lived frequency grating. In other laboratories the information can only be stored once. However, because of the superior phase stability of our laser we can change or reverse the stored information. Phase sensitive detection also enables us to store the information in two orthogonal phases immediately doubling the storage capacity of the material. More importantly we have shown that the orthogonal phases can be used to avoid crosstalk between stored information, a problem that previously made the technique invalid when striving for better signal-tonoise ratio at higher light levels. We have, therefore, been able to show extra capabilities of time domain optical memories and demonstrated the coherent optical processing.

In a further demonstration of the capability of the laser system we have used it to burn a narrow spectral hole over a period of one second in a thin (5 mm) section of highly absorbing (80%) material. Subsequent measurement of the absorption and dispersion associated with this narrow transparency determines that the group velocity of light over the narrow bandwidth is 60 m/s, which is the second slowest on record. The slow group velocity implies a high nonlinearity, and it is this nonlinearity which is employed in the above time-domain optical processing where larger bandwidths are achieved by burning over a wider range of frequencies.

The experimental system has also attraction for more sophisticated spectroscopic investigations of the rare earth transitions themselves. For example, implementation of NMRlike pulse sequences for optical spectroscopy has been an important goal of many groups in Physics and Chemistry for several decades, and we have been able to demonstrate these for the first time. The essential component of the success of this work is the preparation of a narrow spectral feature. This is generated by the application of two overlapped pulses of opposite optical phase. The result is a sharp line of width 25 kHz in a wide spectral hole. Low optical absorption features within this prepared spectral feature are eliminated by the application of a train of π pulses. The consequence of this approach is to enable use of a gated low power frequency stabilized cw laser for successful multi-pulse measurement of the re-formed (image echo) pulse train to obtain dephasing times. The results allow investigation of ion-ion interactions and in the present case have highlighted the effects of the instantaneous spectral diffusion ion dynamics. More importantly the experiments demonstrate that sophisticated NMR-like pulse sequences for isolating specific interactions can be applied to the study of rare earth optical systems. (N. Manson, M. Sellars, G. Pryde)

Diamond Colour Centre Studies

Natural type 2b diamonds contain single substitutional nitrogen atoms. If such a diamond is subjected to radiation damage and then annealed, the carbon vacancies created by the radiation will be trapped by the nitrogen impurities to form a nitrogen-vacancy centre. This centre has been the subject of our studies. There is a ground state spin triplet, and an excited-state spin triplet which gives rise to absorption in the red. The unusual aspect of this centre is that when light is absorbed the ground state becomes spin polarized. This is now considered to arise through a spin selective cross over from the triplet system to a singlet and back to the triplet. The longest wavelength where spin polarization occurs is with excitation at the sharp zero-phonon line, 638 nm. Various holeburning and coherent (Raman heterodyne) measurements can be made at this wavelength. These holeburning and coherent measurements have been observed to vary with magnetic field strength and alignment particularly about an avoided ground state level crossing. Quantitative phenomenological modelling of the spin polarization process this year has highlighted the characteristics and dominance of this mechanism in determining the holeburning and coherence signals. This has enabled us to obtain a better understanding of the centre properties, but the singlet electronic states involved in the spin crossover remains to be established.

The Raman heterodyne magnetic resonance signals associated with the nitrogen-vacancy centre is also used in an entirely different study. The signals are used to study the effects of a strong near-resonance electromagnetic field on an absorbing transition where we capitalize on the exceptional sensitivity of our detection technique. Normally a strong driving field will saturate the system, and measurements of absorption are then too weak to detect. However, in this case we are easily able to detect optical signals in the presence of strong radiofrequency driving fields and we have used this capability for various situations. This year our work centred around experiments where there was more than one saturating field. We concluded a study where there were two driving fields, and also showed that it was possible to get informative data using up to four driving fields. The experiments are in excellent agreement with calculations.

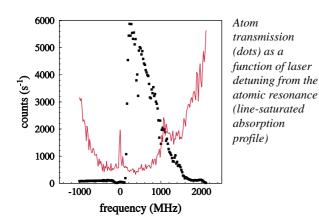
The most recent study involving the same colour centre in diamond illustrated the phenomenon of electromagnetic induced transparency. Here application of an electromagnetic field resonant with one transition can change the absorption of another transition. It is a topic of considerable current interest as it can enable lasing action to be achieved without inversion. Our interest is in the fundamentals of the phenomenon, and our system provides one of the clearest examples of this effect. We have been able to show further that the transparency feature can be split by applying a coherent perturbing field. Electromagnetic induced transparency normally only involves three energy levels and two fields. The transparency can then be split by applying a field at the third transition of such a three level system or by applying a field resonant with a transition between one of these levels and a third level. These effects are shown to have parallels with the Mollow effect and the Autler-Townes effect for driven systems probed by more conventional weak fields. We have experimental data of each of these cases that compare well with calculations of a model system. The calculations can also be extended beyond the range of parameters that can be accessed experimentally. (N. Manson, J. Martin, C. Wei, E. Wilson)

Spectroscopy

A wide range of other specialised optical spectroscopic techniques are employed to study materials. These include laser selective excitation and emission and we have recently completed a study of a potential microlaser material Er doped $KLiF_5$. This work was conducted in conjunction with Professor B. Henderson, Cambridge University, UK and Professor A. Silversmith, Hamilton College, NY, USA.

Together with Dr E. Krausz and Ms R. Purchase (both of the Research School of Chemistry) we have studied electric field and magnetic field effects of zinc phthalocyanine. The particular measurements done in our laboratories were high-resolution

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spectral hole burning which complemented lower resolution holeburning and conventional spectroscopy investigations made in RSC. The studies established that there was a significant dipole induced in the plane of the molecule that was contrary to previous understanding that the only dipole was in the plane.

A holeburning study of rare earth triple chain soaps has also been concluded during the year. The rare earth ion acts as a probe of its local environment and in this study highlighted the glassy structures created by different methods of cooling the soaps. This work was in conjunction with Mr R. Corkery (AM) who obtained his doctorate during 1998.

Another holeburning study has been with Dr H. Reisen (Australian Defence Force Academy) and Dr V. Bursian (Ioffe Institute, St Petersburg). Together we have been investigating the holeburning process in cobalt doped strontium oxide. The dopant in this material substitutes for a host crystal ion but is displaced from the substitutional position. The orientation can be changed by optical excitation and it is considered that this reorientation may provide the basis for a memory device.

We have also been involved with electron spin resonance studies of Si nanocrystals in amorphous silica with Dr S. Choi (Kyung Hee U., South Korea) and Dr R, Elliman (EME). (J. Martin, N. Manson, A. Smith, M. Sellars)

Atom Manipulation

This year the bright metastable helium beam line has been used to extend experiments on atomic wave guiding, as well as being used to load experiments using the magneto-optic trap (see AMPL report). The beam line delivers over 10^{10} atoms/second in the helium $2^{3}S_{1}$ excited state in an area of several square millimetres and with velocities of about a hundred metres/second in the longitudinal direction, and a few metres per second in the transverse direction.

Following the first demonstration of atomic wave guiding for metastable helium atoms in our experiments last year, we have extended these studies to include a range of different hollow fibre geometries and conditions. Using commercially available fused silica capillaries with both round and square cross-section holes ranging from 50 to 10 microns across (see figure 1), we have succeeded in transmitting up to 10,000 atoms/second through the capillaries by using laser light focused into the glass. The evanescent light field thus created on the inside of the fibre wall repels the atoms via the dipole force when the laser frequency is detuned above the atomic resonance frequency (see figure). Without the light field present, the transmitted flux is reduced to around 100 atoms/second when the fibre is perfectly aligned with the atomic beam, and to zero when the capillary is slightly curved.

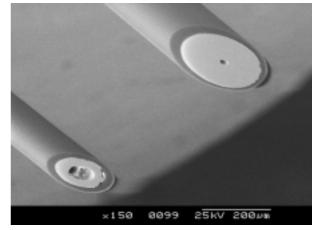
However, it was difficult to improve the transmission efficiency in the presence of laser light above a few percent. This is probably a result of multimode propagation of the laser through the uniform glass capillary, which results in interference on the inside walls of the fibre that allows atoms to strike the wall in the darker regions. To avoid this problem, a single mode fibre was developed that has a stepped refractive index profile around the hole. This fibre was manufactured using special techniques developed by the Optical Fibre Technology Centre in Sydney, part of the Photonics CRC. It is anticipated that the more uniform light field created in this unique hollow fibre will enable much more efficient transmission of the atoms for future experiments in atomic waveguiding. (M. Colla, R. Dall, L. Robinson, J. Swansson, K.G.H. Baldwin; M.D. Hoogerland, S.J. Buckman [AMPL])

UV Laser Spectroscopy

Experiments continued this year on high resolution VUV crosssection measurements of the oxygen Schumann-Runge system near the dissociation limit near 175 nm. These experiments employ four wave difference frequency mixing of high power dye laser radiation in a nonlinear medium (xenon), which we have demonstrated in an international comparison of spectroscopic techniques to yield the most accurate available high resolution cross section measurements for these systems. Currently our best laser resolution is 0.06 cm⁻¹ in the VUV, which is limited primarily by the bandwidth of the dye lasers employed.

A significant improvement in resolution can be achieved by moving to cw injection-seeded pulsed laser systems, which can yield Fourier transform limited laser bandwidths. Such a system employing a seeded dye laser amplifier system was employed in the collaboration between this laboratory and the US National Institute for Standards and Technology which measured the helium 1S-2S two-photon (at 120 nm) transition for the first time. However, even these experiments are limited by chirp induced in the dye pumping process.

We have embarked on a collaborative project with Professor Brian Orr at Macquarie University to develop an injection seeded solid state laser system that may yield improved bandwidth laser radiation for such high resolution spectroscopy studies. This



Electron micrograph of glass capillaries with 40 and 10 micron hole diameters

system uses a cw diode laser to injection-seed an Optical Parametric Oscillator (OPO) followed by an optical parametric amplifier (OPA) which uses periodically poled lithium niobate pumped by the second harmonic of a Nd:YAG laser. Following a successful RIEF proposal with Macquarie University for 1999, we have recently acquired the pump laser for this project and are commencing development of the OPO/OPA system. Establishment of this new high-resolution source should significantly enhance the spectroscopic capabilities of this laboratory. (K. Waring, K.G.H. Baldwin; B.R. Lewis, S.T. Gibson [AMPL])

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Research Accomplishments



Professor George Dracoulis - Head of Nuclear Physics



Nuclear Physics

The Nuclear Physics Department operates the premier laboratory in Australia for accelerator-based research in nuclear physics, providing facilities for national and international users, as well as being the major practitioners in Australia.

Research Summary

The Department's accelerators and other facilities are used for postgraduate and postdoctoral training over a wide range of research, from basic to applied.

The 14UD electrostatic accelerator can 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 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 are used in high-sensitivity applications. This year has seen consistent activity in all research using a variety of beams ranging from deuterons to ¹⁹⁷Au. Higher energies for heavier ions are available from the Linac booster which is being developed to deliver beams to all experimental stations.

The imperatives for basic studies of the nucleus derive from its properties as a quantal, many-body system. Some properties have analogues in macroscopic (classical) systems, whilst others do not. The nucleus is special because while it contains only relatively few particles, it can exhibit both single particle and collective properties from competing motions that are often delicately balanced. The characteristic states can be at comparable energies and in regions of low level density and are thus observable as individual quantum states, which in many cases interfere and mix. The study of such properties falls generally into the province of nuclear spectroscopy whereas the wide range of complex interactions between colliding nuclei is the subject of nuclear reaction dynamics studies. In the latter, since the varied internal nuclear degrees of freedom couple to the relative motion, by both selecting nuclei of different structure and also by tailoring the collision conditions, different aspects of the physical processes can be highlighted. 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 has been developed to span a broad range currently including:

- 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)

The spectrum of research extends from fundamental studies in nuclei to materials analysis, much of it collaborative involving other departments, research schools, universities and institutions. This year again saw extensive use of the facilities by outside users including UK scientists who have formal access through the ANU-EPSRC Agreement.

The ability to carry out such a broad range of research and to maintain international competitiveness, at the same time as providing facilities for other users, relies on a continuing investment in detector instrumentation and accelerator and ion source

technology. As part of the enhancement of research capabilities and accessibility of the facility to outside users, particularly those who may need to install complex detector instrumentation, a more flexible system data acquisition system capable of handling larger multiple-element high-resolution detector arrays and the concomitant high count rates is being developed. This follows a successful bid for funding to the Research Infrastructure, Equipment and Facilities Program (RIEF).

A new fusion product separator based on a superconducting solenoid, is under construction, and should be commissioned late in 2000. The majority of funding for this project was also through an earlier bid to the RIEF scheme. That device will be the basis of extensive measurements by the fission/fusion group. Augmentation of the γ -ray array *CAESAR*, which is the central tool of the spectroscopy pursuit, will also occur over the next two years following support this year from the University Major Equipment Committee.

Considerable disruption occurred during the year as all staff were located in temporary accommodation during a major refurbishment of the department office block. Funding for this and also improvements to some of the technical areas in the Accelerator Building was provided through the University Capital Management Plan.

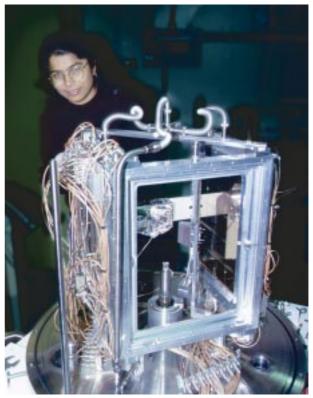
The office block was re-occupied in December. In the longer term, there will also be restructuring of the Accelerator Building to meet the needs of users for detector development and testing, and sample preparation etc. The first "official" function to be held in the new seminar room was a series of scientific talks presented by department staff to mark the retirement of Professor Trevor Ophel. Trevor joined the Department in 1955 as an ANU Scholar and after submitting a PhD thesis in April 1958, spent about eighteen months as a Research Fellow at the Cyclotron Laboratory at Harvard, returning to the ANU in late 1959 as a Research Fellow. Except for a number of periods of extended leave since then, he has been with the Department since, serving as its Head for four years, from July 1988 to July 1992. Trevor will continue in the Department as a Visiting Fellow, from January 1st, 2000.

Details of all aspects of the Department's activities and research studies, some of which are sketched out below, are contained in the Department Annual Report for 1999 (ANU-P/1420), available on request. As well as experiments carried out on the local facilities, each of the research groups has active collaborations with outside groups. In a number of cases, use is made of instrumentation at overseas facilities, complementing our local program.

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.

Research work this year has taken place in a number of complementary areas. These studies are planned to lead to a significant improvement in the understanding of nuclear fusion and fission dynamics, and the interaction between them.



Dr Mahananda Dasgupta with the fission spectrometer

One area of current interest addresses the question of suppression of fusion in reactions initiated by light, loosely-bound projectile nuclei. Experimental data had been obtained in 1998 to compare the break-up of the loosely-bound nucleus ⁶Li to its more strongly-bound neighbour ⁷Li in reactions on ²⁰⁹Bi targets. The resulting fusion cross-sections, which were this year analysed by both ourselves and by our collaborators in Brazil who participated in the measurements, indicate a surprisingly large breakup probability even for ⁷Li, due to the considerable suppression of fusion observed. To complement these results, measurements were carried out this year for a reaction forming the same compound nucleus, but using a projectile that should not be susceptible to break up. This should allow confirmation of the fusion suppression for 7Li. This work has implications for fusion reactions with unstable nuclei, being planned for new radioactive beam facilities.

Another aspect of recent studies involves the measurement of fission angular anisotropies. These give a unique insight into fusion and fission reactions because the anisotropy is determined by the most compact shape in which the combined nuclear system finds itself, after the decision to fission. It is the observable most influenced by the dynamical processes occurring during the fission of hot nuclei. Systematic measurements of anisotropies for reactions with targets having significant groundstate spins were also initiated, and a detailed study on the influence of entrance channel mass-asymmetry on fission dynamics has almost been completed. Precise measurements of anisotropies were carried out to investigate the suggestion that there may be a memory of the shape of the target nuclei maintained throughout the reaction process. The results have shown that such memory effects (as we anticipated) are restricted to collisions forming very heavy compound nuclei, where there is a high Coulomb potential.

Even in more conventional cases, some surprises have emerged. Drawing on a comprehensive analysis of our precise measurements of the fusion cross-sections for the reaction of ¹⁶O with ²⁰⁸Pb, we have shown decisively that the standard shape of the nucleus-nucleus potential cannot describe the data at both near-barrier and sub-barrier energies. Measurements to investigate this effect were carried out by the Group last year at the Argonne National Laboratory. Vital follow-up measurements at the ANU were successfully carried out this year, of extremely small fusion yields, at deep sub-barrier energies, to investigate the quantum-tunnelling probabilities. Data analysis is in progress. Further measurements designed to probe in more detail the shape of the nucleus-nucleus potential are in progress.

Part of the research program planned for the next few years will use the RIEF funded Unique Separator for Fusion Products, currently being constructed. Considerable work this year went into a close collaboration with the manufacturer to obtain a device matching our requirements. Delivery is expected early in 2000.

Nuclear Spectroscopy

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

The broad program of spectroscopic studies over a wide range of nuclei has continued this year, including the study of relatively neutron-rich well-deformed nuclei. The main emphasis in these was on the completion of experimental studies on the lutetium nuclei whose spectroscopy will contribute to the understanding of the systematics of single-particle states and the competition between single- and multi-quasiparticle states and their collective motions. This work, as well as new studies of ytterbium nuclei, and results on hafnium nuclei, such as ¹⁷⁹Hf, have exploited the particle-detector-ball and incomplete fusion reactions with relatively light projectiles.

Studies of the coupling between rotational and intrinsic degrees of freedom have also been pursued in the guise of the measurement and interpretation of the rotational motion in multiquasiparticle states, in which orbital blocking affects quantities such as the collective magnetic moments, because of a reduction in pairing. Searches have also begun for the predicted "chiral" bands in γ -asymmetric nuclei, and further studies are being carried out, initially in the odd-odd iridium nuclei, to elucidate the role of residual proton-neutron interactions in causing anomalous signature splittings.

Our activities in the study of shape co-existence in very neutrondeficient lead nuclei have also continued with the identification and characterisation of isomers in ¹⁸⁸Pb and related studies of ¹⁸⁷Tl, carried out in collaboration with the Jyvaskyla Group. The ¹⁸⁸Pb case includes a proposed two-quasiparticle, $K^{\pi} = 8^{-}$ excitation whose existence provides independent evidence that the potential sub-minimum is prolate in shape.

In the area of instrumentation we have continued development of the electron-detector array, *HONEY* which will be used in the superconducting solenoid for broad-range electron-electron coincidences, particularly of very heavy nuclei. Following a number of evaluation runs, further technical improvements are planned. Improvements were also made to a new compact electromagnet commissioned for in-beam g-factor measurements in *CAESAR*. It has now been used for the first of an extensive set of measurements aimed at exploiting angular correlation techniques for the in-beam measurement of the g-factors of short-lived states, implanted into ferromagnetic hosts.

Magnetic Moments and In-beam Hyperfine Interactions

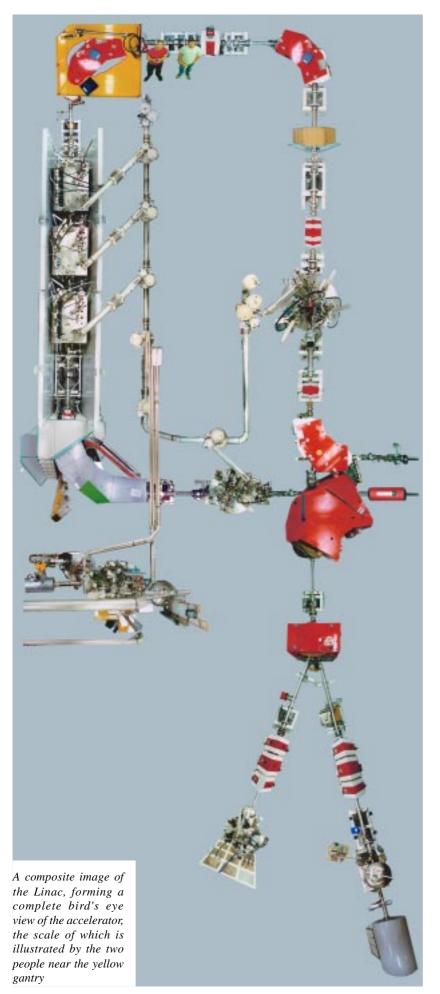
The large angular and linear momenta involved in heavy ion reactions is used to facilitate various techniques to study nuclear structure or to probe atomic environments.

This research program has continued to study a broad range of physical phenomena related by the theme of in-beam hyperfine interactions, with the completion of long-term projects and the launch of new projects.

One aspect that has come to fruition follows the measurements, over a number of years, of the magnetic moments and lifetimes of low-excitation states in the iridium isotopes ¹⁹¹Ir and ¹⁹³Ir. Two aims were in view: firstly, the use of these nuclei to probe the time-variation (on the picosecond timescale) in the fields around implanted nuclei; and secondly, the exploration of the internal structure of the nuclei themselves. The first aim was realised in the results of the studies of pre-equilibrium effects in hyperfine fields due to the implantation of iridium into iron, which were completed this year and published in Physical Review Letters. The second aim has resulted in collaboration with colleagues in the Department of Theoretical Physics and at GANIL, in France, to interpret the structures of the nuclei ¹⁹¹Ir and ¹⁹³Ir in terms of supersymmetry models. Although the excitation energies of these nuclei can be described by simple and elegant supersymmetry schemes, the measured magnetic properties show that the nuclei are in fact much more complex.



Rendered view of the entrance cone of the superconducting solenoid separator, machined by Miro Peric in the School's Mechanical Workshop



On the experimental side, the major focus this year has been on the implementation of a new technique to measure magnetic moments in unstable nuclei. The technique exploits the perturbations of Directional γ - γ Correlations from reaction Oriented (DCO) nuclei measured by the CAESAR array. It is new in that it uses the coincidence relations between correlated y-rays emitted from excited nuclei to select a state of interest from a complex spectrum of states populated following a heavy ion induced reaction. Following preliminary measurements in 1998, data have now been taken for the neutron-deficient platinum isotopes 180Pt, ¹⁸²Pt and ¹⁸⁴Pt and for several nuclei in the mass-80 region. The theory required to evaluate the data has been formulated, and computer programs are being written to analyze the cases of immediate interest. This work is being performed in association with the Nuclear Spectroscopy Program.

Perturbed Angular Correlations and Hyperfine Interactions in Materials

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

The emphasis of current work in the application of the Perturbed Angular Correlation (PAC) method to the study of semiconductor materials has been in the area of ion-beam induced amorphization of Ge. This work follows on from measurements of amorphization and relaxation processes in indium phosphide that have been published this year in Applied Physics Letters. The PAC measurements have been performed as part of a broader study that includes both Rutherford Backscattering (RBS) and Extended X-ray Fine Structure (EXAFS) measurements.

In the PAC measurements samples were prepared by pre-implantating ¹¹¹In via a direct production/implantation technique using beams from the 14 UD accelerator. Following rapid thermal annealing, amorphization was achieved using Ge beams from the EME Implanter at energies chosen to reproduce the depth distribution of the ¹¹¹In. Implantation doses were between 2×10^{12} and 5×10^{15} ions/cm².

As in the measurements with InP, a differentiation into fractions associated with highly damaged amorphous and disordered environments could be achieved. In addition, the measurements also distinguished two well-defined interaction frequencies resulting from point defects being attracted to the In ion. While these frequencies have been seen in previous studies of damage induced in Ge, the fractions of defects at probe sites are not in accord with previous descriptions. Work is continuing in this area.

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 continued unabated throughout 1999, and was spread across a broad spectrum of isotopes and fields of application. The latter ranged across biomedicine, dating of ancient human sites in Australia, meteoritics and a variety of environmental tracing applications.

The collaboration with the University of Manchester was concentrated on exploitation of the new technetium-99 capability. Three different projects are underway: a gut uptake study on a human subject in order to define the long-term retention of technetium, a time-series of seaweeds obtained from the archives of an alginate producer in Norway in order to study the impact at this Scandinavian site of releases of ⁹⁹Tc, and finally, a pilot study of the distribution of ⁹⁹Tc among different molecular-weight components of seaweed, whose aim is the determination of the mechanism through which seaweeds concentrate technetium.

Another pilot study last year of plutonium releases from the Mayak plutonium production plant in the Urals region of Russia

highlighted the need for a better understanding of the mechanism of plutonium transport in river water. Further studies this year in collaboration with the Agricultural University of Norway have shown that most of the plutonium is carried by fine suspended sediment, and only a small fraction is actually in solution. In addition, the isotope ratios of this plutonium are not consistent with the previously postulated source, indicating that plutonium is coming from areas other than that contaminated by the extensive early releases from the plant. Biomedical applications of plutonium include a study of the long-term retention by humans and measurement of the uptake of plutonium from inhaled dust. The former, which is a collaboration with AEA Technology at Harwell and Middlesex University, is showing that Pu levels fall for the first year after dosing but are approximately constant thereafter. Recommended limits of plutonium uptake may need revision in the light of the present results.

Considerable effort also went into ¹⁰Be in the course of the year including a new project on landscape denudation and sediment storage, initiated in collaboration with RSES. This project exploits the ¹⁰Be produced in quartz at the Earth's surface. In contrast, another project in collaboration with CRES uses the ¹⁰Be produced in the atmosphere and washed out in rainfall in a detailed study of an undisturbed hill slope south of Canberra. This study aims to estimate historical rates of erosion in this landscape. In addition, measurements on glacial moraines in the Snowy Mountains and Tasmania (a collaboration with the University of Washington and RSES) have been completed and are providing important data on the timing of the last glacial maximum in the southern hemisphere.

There has also been considerable activity on the ¹⁴C dating front, where the highlight has been the first secure radiocarbon date of greater than 40 ka for human occupation of Australia. Dates from other techniques such as Optically Stimulated Luminescence (OSL), Electron Spin Resonance (ESR) and U/



The control room for the 14UD and Linac accelerators

esearch Accomplishments (Nuclear Physics) Th dating have been pointing for some time to earlier occupation, but this is the first positive confirmation from radiocarbon dating. The site is Devil's Lair, a cave in the Margaret River region of Western Australia, and dates on charcoal associated with human artefacts point to human occupation of the area from at least 46 ka before present. This work is a collaboration with RSES, and builds on new procedures for reducing contamination of charcoal which have been developed over the past 18 months.

Chlorine-36 continues to be one of the more important isotopes. The year has seen the publication of two papers on groundwater resources in arid central Australia. One shows that deep water in the Mereenie sandstone aquifer, which supplies Alice Springs, is older than 500 ka, indicating that flow rates in this aquifer are extremely low. The other was a component of the Western Water Study which has been determining the size and quality of the groundwater resources in traditional Aboriginal lands in the southwest of the Northern Territory. It appears that major recharge of the aquifers in this region occurs only at times of relatively high rainfall such as the Holocene and the previous interglacial period at 120 ka before present. A major report on the Great Artesian Basin has also been completed. This incorporates 300 ³⁶Cl measurements that have been accumulated over several years.

New developments included the first measurements by AMS of ³²Si in natural samples, in this case rain, snow and ice from New Zealand. This work, which is a collaboration with Geological and Nuclear Sciences in New Zealand and aims to date ice in the difficult 100-1000 year time range, breaks new ground in handling and measuring fewer than a million atoms of ³²Si. Iodine-129 measurements have also been revived in order to shed light on the origins of the wide variability among different laboratories in a recent inter-laboratory comparison exercise.

Heavy Ion Elastic Recoil Detection Analysis (ERDA)

Toward absolute 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.

Heavy ion Elastic Recoil Detection Analysis (ERDA) is a technique whereby constituent elements of thin films, ejected by the scattering of high energy, heavy ion beams, are detected and identified to provide direct stoichiometric composition and the depth profiles of each of the elements. Under favorable circumstances, elements ranging between hydrogen and gold can be analyzed simultaneously. Following instrumentation developments in the previous year, the ERDA program operated routinely, embracing a wide variety of samples provided both by sections of the School and by external laboratories. Considerable emphasis was directed toward demonstrating that hydrogen could be detected with the large acceptance gas ionization detector, rather than by the usual, but less satisfactory, method involving small surface barrier detectors. Hydrogen depth profiles were obtained either by using incident beam energies low enough to allow the recoil protons to be stopped in the detector, or from the energy loss distributions of transmitted protons where higher beam energies were used. The former method provides superior depth resolution for hydrogen, though identification and separation of the heavier elements is somewhat poorer at the lower beam energies required. Samples measured included nitrided stainless steel from the University of New England and a series of high temperature superconducting films prepared by the CSIRO at Lindfield.

The same superconducting films were investigated to examine beam-induced sample modifications and to compare the Y/Ba/Cu stoichiometries found using ERDA with those from RBS measurements made with 2 MeV alpha particles and 56 MeV²⁸Si ions. Structural modifications of the superconducting films by the ¹⁹⁷Au beams used for the ERDA measurements are evident from RBS channelling measurements. More obviously, the normally opaque films become transparent after bombardment. Nonetheless, it was found that compositional changes, in particular that of oxygen, were insignificant. Consistency was obtained for the three analysis techniques that were used.

On the technical side, a major effort has been made to establish the magnitude and nature of the pulse height defect for very heavy ions in the detector stopping gas. The fraction of the energy lost by ions in the gas that is detectable as electron-ion pairs, varies significantly with ion mass. Almost constant for masses up to about 40, this fraction decreases for larger masses so that the measured energy/MeV for 100 MeV ¹⁹⁷Au ions is about 12.5% less than that for 50 MeV²⁸Si. Extensive data have been obtained for a number of ion species between ¹²C and ¹⁹⁷Au with measurements spanning a wide range of energies. Careful measurements of the energy lost by the various ions in the entrance window were an essential part of the study. Preliminary indications are that the pulse height defects in gases are little different from those previously found for silicon, even though the linear ionization density is much lower.

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Professor and Head of Department G.D. Dracoulis, BSc PhD Melb, FAIP, FAPS, Hon. FRSNZ, FAA

Professor T.R. Ophel, BSc Adel, PhD (until December)

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Reader

A.P. Byrne, MSc Auck, PhD, FAIP (joint appointment with Dept Physics, The Faculties)

Senior Research Fellow T. Kibédi, PhD Debrecen

Research Fellows

R.A. Bark, BSc Melb, PhD R.G. Cresswell, BSc Sheffield, MSc PhD Toronto S.M. Mullins, BSc Leicester, DPhil York, MAIP (until July)

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Dr H. Timmers, DipPhys Munich, PhD, MAIP, MDPG (joint EME, Dept Physics and Theoretical Physics) (from July)

Post Doctoral Fellows

P.A. Hausladen BA Williams, PhD Penn (from April) C.R. Morton, BSc Sydney, PhD, MAIP A. Mukherjee, BSc MSc PhD Calcutta (from November)

Visiting Fellows

Dr M. di Tada, MSc, PhD Buenos Aires (until December) Dr G.M. dos Santos, CNPq, Universidade Federal Fluminense, Brazil, (25 May 1999 - 24 May 2000) Ms R.G. Liberman, Laboratorio Tandar, Argentina, (10 July - 27 December) Dr S.M. Mullins, BSc Leicester, DPhil York, MAIP (1 Oct 99-28 Jan 2000) Professor J.O. Newton, MA PhD Camb., DSc Manc., FAA

Professor R.H. Spear, PhD DSc Melb, FAPS, FAIP Professor S.R. Taylor, MSc NZ, PhD Indiana, MA DSc Oxf FAA Hon. FGS, Hon. FRSNZ (Emeritus Professor) Dr H. Timmers, DipPhys Munich, PhD (joint EME) (until June) Mr A.A. Tulapurkar, Tata Inst. Fundamental Research,

Accelerator Research and Operations Manager D.C. Weisser, MSc PhD Minn, FAIP

Research Officer

G.S. Foote, BSc Lond, PhD

Mumbai, India, (10 May - 31 July)

Engineer

N. Lobanov, BSc Moscow, PhD St Petersburg

Technical Officers

J. Bockwinkel, AssocDipMechEng A.K. Cooper, AssocDipMechEng G.J. Gilmour, DipArtsPhotography CIT (until November) A.B. Harding J. Heighway, AssocDipAppSci J.M. Kennedy L. Lariosa A.G. Muirhead A.J. Rawlinson R.B. Turkentine H.J. Wallace

Departmental Administrator M. O'Neill



Research Accomplishments



Professor Allan Snyder - Head of Optical Sciences



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

Optical Sciences Centre

The Centre performs both fundamental and applied research in the exciting and rapidly expanding fields of nonlinear physics and nonlinear optics, including: light-guiding-light. spatial solitons. creating optical components with light. linear and nonlinear guided wave optics. nonlinear properties of magnetic films. photonic crystals and waveguides. the dynamics of nonlinear lattices. Bose Einstein condensates. optical nanostructures.

These subjects are at the hub of contemporary science with a multitude of potential spin-offs to the latest technologies.

Research Summary

This was a fruitful year with research commencing in many new directions, and a number of great achievements. Firstly, Professor Synder and Dr Ladouceur's dream of virtual circuitry; a transparent cube with a myriad of interconnections, created, maintained and arranged by light itself, became the March cover story in Optics and Photonics News. Secondly, the Optical Sciences Centre (OSC) had eight papers published this year in Physical Review Letters. Finally, for the fourth year in a row, three projects of our research were chosen for publication in the special December issue of Optics and Photonics News to represent the important advances of the year in optics across the globe. This is really a great achievement that confirms our world-leading position in the field of guided wave optics and nonlinear physics.

This year due to recent changes in our global strategy of research activities in nonlinear physics at OSC, and our success in gaining additional funding (\$600k) via the Performance and Planning Fund (PPF) scheme of the Institute of Advanced Studies, the OSC has extended the frontiers of its research into exciting new areas of nonlinear physics. In addition, because of the leading international role of our group and following a number of key results published in previous years, we have attracted many international visitors and students this year. In 1999 the Centre hosted four long-term visitors (from Japan, Spain, Ukraine, and Indonesia) and four international research students (from France, Sweden, and Germany).

Current OSC research projects are devoted to new concepts in linear and nonlinear guided wave optics; light guiding light; long-distance optical communication and wavelength division multiplexed (WDM) systems; bit-parallel optical fibre networks and systems; linear and nonlinear photonic crystals; nonlinear spin dynamics in magnetic films; pulse propagation in active optical fibers; self-trapping and guided waves in nonlinear optical wave guides; the theory of frequency mixing and parametric processes in waveguides; the dynamics of atom lasers; and Bose-Einstein condensation.

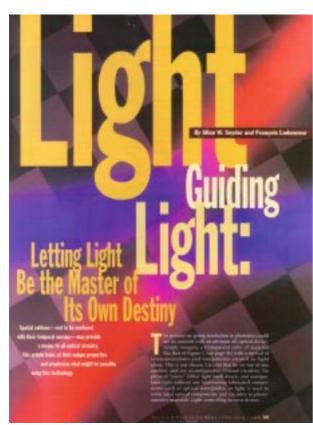
Our work provides the basis for new experimental studies carried out both here at ANU and elsewhere in close collaboration with other leading national and international groups. Several important projects were carried out either together with experimental groups, or were closely connected with experimental results and their theoretical explanation. The Centre is one of the key players in the Australian Photonics Cooperative Research Centre.

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

Spatial Optical Solitons and Light Guiding Light

Spatial optical solitons is one of our traditional topics of research, with a number of different projects involving collaborations with overseas institutions including CREOL (USA), Princeton University (USA), University of Glasgow (UK) and Technion (Israel). This research includes the analysis of the existence and stability of solitons, the self-trapping effect, transverse instabilities and other problems of light guiding light. This

Research School of Physical Sciences & Engineering 1999.



Cover story of Optics and Photonics News, featuring the work of the Centre

year, among our major highlights is the cover story of Optics and Photonics News on the dream of virtual circuitry, the stability theory for multi-component vector solitary waves and the first demonstration of stability of multi-hump solitons, the theoretical explanation of soliton spiralling in a bulk, further confirmed by experiments, the prediction and observation of multi-soliton bound states and finally a comprehensive theory of soliton transverse effects. A major review paper has been completed during 1999, *Self-Focusing and Transverse Instabilities of Solitary Waves* by Yu. Kivshar and D. Pelinovsky, and will appear in Physics Reports. (*E.A. Ostrovskaya, Yu.S. Kivshar, A.W. Snyder; D. Skryabin, W. Firth [U. Glasgow]; M. Segev* [*Princeton U.J*)

Incoherent Solitons

After the recent discovery of self-trapping of incoherent light and the so-called incoherent spatial solitons, the study of selftrapped incoherent beams became one of the hottest research topics in nonlinear guided-wave optics. Recent achievements of the members of our group include the analysis of classes of exact solutions of multi-component nonlinear systems and the study of incoherent effects in collapse dynamics. In part, this work was carried out in close collaboration with the research team of the Laser Physics Centre. (*N. Akhmediev, A. Ankiewicz, A.A. Sukhorukov, D. Edmundson; W. Krowlikowski [LPC]; O. Bang [Technical U. Denmark]*)

Cascaded Nonlinearities and Quasi-phase-matching

After the discovery of cascaded nonlinearities of noncentrosymmetric optical materials several years ago, the OSC remains among the leading groups in this field. Our most recent results are in the theory of quasi-phase-matched structures where phase matching and enhancement of the parametric effects is achieved by the manufactured periodic systems of domains (grating). This year, our major results include the new concept of parametrically enhanced nonlinearities – multi-step cascading; the first prediction of a new object in physics – the quasi-periodic solitary wave; and a comprehensive theory of parametric optical vortices. (Yu.S. Kivshar, A.A. Sukhorukov, T.J. Alexander; O. Bang, P. Christiansen [Technical U. Denmark]; S. Saltiel [Sofia U.])

Pulse Propagation in Optical Fibres

Stable polarisation-locked temporal vector solitons in optical fibres have been analysed in the context of mode-locked fibre lasers with a saturable absorber. The phase-locked temporal solitons have been a subject of several theoretical works and they have been recently observed experimentally by a collaborative research team from Bell Labs, Colorado, and Australia. (*N. Akhmediev; S.T. Cundiff, B.C. Collings [U. Colorado]; W.H. Knox [Bell Labs]*)

Nonlinear Effects in Magnetic Films

Our long-term collaboration with several research groups working on the nonlinear dynamics of magnetic systems (e.g. magnetic YIG films) resulted this year in several important discoveries, such as the first analytical explanation of the anomalous generation of spin-wave dark solitons in magnetic films, and the first observation of the spin-wave self-focusing



Dr Elena Ostrovskaya, winner of the inaugural Jagadishwar Mahanty Prize for her thesis, Optical Vector Solitons

carried out by different experimental methods in Germany and the US, where our role was the development of the corresponding nonlinear theory. (Yu.S. Kivshar, E.A. Ostrovskaya; A.Slavin [U. Oakland]; O. Buttner [Technical U. Darmstadt]; H. Bener, B. Hillebrands [U. Kaiserslanten]).

Nonlinear Photonic Crystals and Discrete Models

The concept of photonic band gap materials was first suggested about 10 years ago and, due to recent progress in technology, such photonic band gap materials are now considered as a new generation of optical materials --- "the semiconductors of the future", that offer a number of unique properties in wave transmission. So far, these properties have been analyzed for the linear regime assuming that the field amplitudes are small. However, photonic band gap material that involves nonlinear properties will be the most attractive of the next generation of nonlinear materials and nonlinear all-optical switching devices. The properties of nonlinear photonic band gap crystals can be manipulated by introducing defects due to impurities. Recently, we have revealed a number of intriguing properties of nonlinear impurity modes in photonic crystals with quadratic nonlinear response of nonlinear interfaces. These results have been highlighted in a special issue of Optics and Photonics News (Optics '99). (A.A. Sukhorukov, Yu.S. Kivshar; O. Bang [Technical U. Denmark])

Bose-Einstein Condensates and Nonlinear Atomoptics

Since 1995, when Bose-Einstein Condensation (BEC) was first demonstrated experimentally, the number of interesting phenomena to be explored in this field is still growing rapidly. We started a completely new direction in this field, applying our expertise gained in guided-wave optics to analyze the dynamics of matter waves in a trap. We entered the BEC field several months ago, and already have three papers accepted or submitted. In collaboration with the group from Dept. Physics in The Faculties (Dr Craig Savage), our team also works on the theory of atomic lasers, and organized an international workshop in November. (*T.J. Alexander, Yu.S. Kivshar, E.A. Ostrovskaya; C. Savage [Physics, The Faculties]; D. Anderson, M. Lisak* [Chalmers U. Technology]).

Linear Optical Devices

A wide range of devices for manipulating and processing light has been investigated, including tapered multimode planar waveguide taps, multi-wavelength add/drop planar gratingassisted couplers, metal-clad tapered fibres for microscopy, and multimode liquid-core fibres for sensing applications. Transient effects in buried channel waveguides have been quantified and photonic crystal effects on propagation modelled. The radiative behaviour of tapered fibres has been investigated both theoretically and experimentally, and the profile of fused taper couplers measured and modelled. Sophisticated software now enables the accurate modelling and design of either single devices of a chain of devices, as a service to groups in the School and within the Australian Photonics Cooperative Research Centre. (J.D. Love, A. Ankiewicz, S. Ashby, R. Jarvis, S. Tomljenovic-Hanic, K. Gaff; P. Moar, B. Gibson, J. Katsifolis, [La Trobe U.]; A. Ash [RMIT]).

Novel Silica-based Materials

In collaboration with the Space and Plasma Processing Group in the Plasma Research Laboratory (PRL) and the Laser Physics Centre, a new range of doped silica materials with particularly low hydrogen content is being developed. The material is produced in the PRL Helicon Activated Reactive Evaporation machine and characterized as the precursor to the fabrication of a range of planar devices which are predicted to exhibit low loss over the whole available spectrum for optical fibre communications. (K. Gaff, R.A. Jarvis, J.D. Love; R.W. Boswell [PRL])

Future Directions

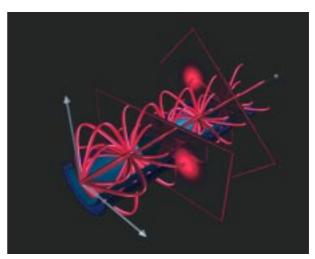
Nonlinear models of Biophysics

Supported by PPF funds, we have started to pursue our research on nonlinear systems into new exciting areas, including biophysics. It is naive to think that such research can be started without proper expertise. That is why, to achieve our goals, we have invited several experts to present lecture courses. Our possible research direction might be the dynamics of proteins and nonlinear models for molecular motors. The first visitor, Professor J.A. Tuszynski, will give three lectures in March 2000.

During the last months we have developed collaborative links with several research groups in biophysics in order to correctly identify possible directions for our research in the future. Our expertise seems to be very compatible with the current research activities in biophysics and we observe a mutual interest in such collaborations. In particular, Professor Kivshar has been invited to present an overview of nonlinear lattice dynamics and selftrapping in discrete nonlinear chains at the meeting "Biophysics and Biochemistry of Motor Proteins" (Banff, Canada, August 27-September 1, 2000).

Bit-parallel Wavelength Division Multiplexed (WDM) Fibre Optics Links

Recent rapid progress in high-speed communication and computing calls for the development of a radically new approach to increase the speed of computer interconnects. We have developed new concepts for bit-parallel WDM pulse transmission for a fibre optic supercomputer interconnect, which is a single-



Computer model of an incoherent soliton

mode analogue of the optical ribbon cable, based on multifrequency pulse-alignment in single-mode optical fiber links. This concept will be further developed (and also verified experimentally) in collaboration with the Jet Propulsion Laboratory of NASA (Pasadena, USA) and is expected to bring commercial partners and patents.

Nonlinear Physics and Geometry

Condensed matter systems of nontrivial geometry are becoming increasingly prevalent as we move to study low-dimensional nanoscale systems such as nanotubes, microtubules, electronic and photonic waveguide structures, and other mesoscale physical and biophysical systems. Geometry in such systems manifests itself in creating linear quasi-localized or bound states. We wish to pursue another concept analyzing the geometry-induced enhancement of nonlinear properties. Indeed, nonlinearity itself usually leads to energy localization. Acting together, these two mechanisms are expected to bring many interesting and unexpected effects that we hope will explain many new properties of nonlinear mesoscale physics. One of our current visitors, Dr S. Mingaleev, is currently working in this direction.

STAFF

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Professor and Deputy Head Y.S. Kivshar, PhD USSR Acad Sci, FAIP

Professors

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Research Fellows

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Visiting Fellows

- A. Buryak, ADFA
- D. Edmundson, Simon Fraser, Canada
- T. Iakeshi, Ehime University (from June)
- A. Hughes, National Vision Research Inst.
- W.S. Jagger, Monash University
- F. Ladouceur, Virtual Photonics Incorporated S. Mingalev, Bogolyubov Institute for Theoretical
- Physics (from October)
- E. Ostrovskaya, RSPhysSE (from October)
- R. Vance, Virtual Photonics Incorporated
- F. Zen, Bandung Institute of Technology (from July)

Departmental Administrator

A.G. Robins



Research Accomplishments



Professor Jeffrey Harris - Head of Plasma Research Laboratory



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 consists administratively of two groups: the Toroidal Group and the Space Plasma and Plasma Processing Group (SP³). 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 J.H. Harris is Head of the Laboratory and the Toroidal Group, Professor R.W. Boswell leads the SP³ group, and Professor R.L. Dewar leads the Plasma Theory group.

The Laboratory conducts both fundamental and applied research into the properties of ionized 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 the collaborative linkages among its three component 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 understanding of the behaviour of plasmas, which are complex systems far from thermodynamic equilibrium, poses a fundamental challenge in experimental and theoretical physics. A great range of physical expertise is called upon to produce, diagnose and model magnetically confined plasmas, making it a fruitful area for research. The Laboratory has thus attracted 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 research areas is in fusion energy and plasma processing of materials. Fusion power offers the potential for large-scale electricity generation using reactions like those that power the sun and stars, in which light nuclei, particularly hydrogen isotopes, combine to form heavier nuclei. The attraction of fusion is its light atom fuel cycle (based ultimately on water) and low emissions of atmospheric pollutants and gases such as CO_2 which contribute to global warming. In the long term, fusion could be important in base load power generation, but it poses challenging problems both in plasma physics and materials science. These are being addressed in a worldwide research program, with the largest experimental devices in Japan, the United States, and the European Union. The Plasma Research Laboratory has pioneered the development of the heliac concept, for containing hot plasma in an externally produced helical magnetic field. It has built a large experimental realization 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 operative 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.

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

Research School of Physical Sciences & Engineering 1999-

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. Further development of the plasma antenna for ship-borne applications will now proceed.

The WEDGE low-cost virtual reality theatre continues to enjoy great popular success (a WEDGE is installed in the Powerhouse Museum in Sydney) and numerous inquiries are received from organizations interested in setting up virtual environments for research and education.

These developments and others are described in more detail in the sections below and on the PRL web site.

Development of the H-1 National Facility

The major activity for the Toroidal Group in 1999 marked the completion of the main upgrades to the H-1 National Facility. This, the second round of upgrades, included installation and commissioning of a new magnetic field power supply, switchgear and patch panel, vacuum upgrades including 26 additional or upgraded access ports and a cryopump, and commissioning of the electron cyclotron heating system as part of the collaboration with Kyoto University and the Japanese National Institute for Fusion Science (NIFS). Because the facility now has a degree of redundancy in power, heating and vacuum systems, the

remaining upgrades to heating and launching systems and bringing the machine up to full magnetic field (1 Tesla) will result in much smaller interruptions to operation over the next two years.

The new power supply will increase the magnetic field of the H-1NF device from its present operating value of 0.2 T to its design value of 1 T, and was successfully tested up to 0.6 Tesla into the heliac coil set, in preparation for operation at 0.5 Tesla for the first year. Comprehensive tests showed very stable programmable constant current into H-1NF up to 8,500 A, with variations of a small fraction of one ampere. This ensures highly accurate magnetic geometry as well as avoiding interference with measurement systems, and any induction of current into this inherently current-free plasma configuration. These tests applied large electromechanical forces to each magnetic field coil (of the order of tonnes) but the subsequent motion of the coils was limited to 1 mm, in general agreement with finite element stress calculations.

A secondary supply powers the control windings and allows the plasma shape to be varied under computer control over a much wider range than other plasma configurations, with the option of varying the current during a plasma pulse. The supplies delivered full rated current (14,000 A) and voltage (Main supply: 800 V, Secondary supply: 100 V) into a test load, and demonstrated controlled switch "on" and "off" to minimize mains disturbances. 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" capable of carrying 14,000 A for two seconds. Relevant information including total winding inductance, mutual inductance and resistance is passed on to the power supply controller. This enables full exploitation



The outer vacuum jacket is carefully lowered onto the H1-NF after an upgrade

of the wide range of magnetic characteristics accessible to the H-1NF.

Credit for the success of this ambitious and unique project, combining a power plant similar to that powering a "very fast train", with the precision and flexibility of a laboratory instrument, is due to a wide range 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).

The main benefit of the vacuum upgrade is the installation of 16 additional ports for users to connect experiments to the H-1NF. Many of these have gate valves allowing changeover without vacuum interruption. The modifications to the vessel, including the welding of several large vacuum ports (up to 600 mm), were performed very professionally by Cowan Engineering of Gosford. A cryopump will allow rapid pumpdown after a vacuum break, and the vacuum test stand will be useful for preparing new experiments for connection to the facility, especially for visiting experimentalists. Many modifications for high power operations were made, including protective electrical components, fixed plasma limiters and a fast moveable tubular limiter. This device will be automatically inserted into the plasma volume to prevent the generation of runaway electrons when the magnetic field is changed quickly. The development of the H-1NF heating system is also progressing. The waveguide line and vacuum transmission window connecting the 200 kW, 28 GHz, Kyoto/NIFS gyrotron to H-1NF have been assembled and tested prior to the first heating experiments. A new RF antenna and DC block have also been manufactured.

Many diagnostic systems were installed or upgraded when H-1NF was shut down, including a 55 channel fibre-optic rotating wheel for vector tomography; a 2-mm scattering system to be used for turbulence studies; a MOSS camera for ultra-high resolution spectroscopic imaging; and a "camera" for imaging soft X-ray emission.

Toroidal Plasma Physics

Turbulence, Transport and Effects of the Electric Field

Fluctuations and the turbulence-driven particle and energy transport within the plasma are among the most important fundamental problems in the physics of the magnetic confinement of plasmas. Instabilities and turbulence contribute to the particle and energy loss across the magnetic fields in the H-1NF heliac as well as in other toroidal plasmas. Sheared plasma flows are thought to modify the turbulence, although the details of this modification at the microscopic level are not yet understood.

Recent results from H-1NF indicate that shearing only the flow of the electron fluid in the plasma, without any significant mass (ion) flow being present, can modify the turbulence-driven particle transport. This conclusion makes the prospects of achieving efficient high confinement in stellarators more optimistic. A high "magnetic viscosity" of the stellarator plasmas slows down the bulk plasma rotation, but this does not seem to be a problem for the turbulence reduction.

Another important result is that the sign of the shear (radial derivative) in the radial electric field is crucial for the way in which the turbulent transport is modified. It has been shown that under certain conditions the particle flux can even be radially reversed improving the particle confinement. To take advantage of this practically important result, several new experiments on the formation of the radial electric field in H-1NF and a number of the fluctuation-related plasma diagnostics (see below) are being set up on the H-1NF heliac. (*M.G. Shats, W. Solomon, H. Punzmann, D.L. Rudakov, J.H. Harris*)

http://rsphysse.anu.edu.au/~mgs112/html/transport.htm

Electron-Cyclotron-Resonance Heating (ECRH) of Plasma in H-1NF

A gyrotron, a high power microwave source, generating 200 kW at 28 GHz is used in the H-1NF heliac for plasma production and heating at higher magnetic fields (0.5 and 1.0 T). The microwave power is absorbed by the plasma electrons that gyrate in the strong magnetic field in resonance with the oscillating electric field produced by the gyrotron.

Among the advantages of this heating method is good spatial localisation of the power deposition. The heating region can also be easily and finely controlled by tuning the magnetic field in H-1NF. This gives a number of new experimental opportunities to study fundamental plasma effects, including the electron transport in H-1NF and the formation of radial electric fields.

A microwave transmission line that connects the gyrotron with the plasma includes mode converters, transforming the circularly polarised microwave radiation of the gyrotron into a linearly polarised Gaussian beam. The beam then propagates quasi-



A composite panorama of the interior of H1-NF, this is viewable as an animated virtual reality panorama at http://rsphysse.anu.edu.au/admin/photos/Plasmamovie.html - the closest thing to standing inside H1-NF

optically inside a corrugated waveguide. Two reflecting polarisers supplied by Kyoto University, Japan, finely control the polarisation of the microwave beam. The microwave beam is then launched into the H-1NF vacuum tank and focussed into the plasma using in-vacuum quasi-optical mirrors. The transmission line has been bench-tested and will shortly be commissioned in a high power test on the H-1NF heliac.

http://rsphysse.anu.edu.au/~hop112/ECRH.htm

A new ray tracing code has been developed to study the propagation, absorption and the power deposition profiles during ECRH in the H-1NF. Initial modelling results indicate that a single pass absorption can reach up to 90% of the launched power and the power deposition profiles are narrow (less than 0.2 of the plasma radius). The expected plasma parameters with ECRH at 0.5 T are as follows: electron density $n_e < 4x10^{18} \text{ m}^{-3}$; electron temperature $T_e \sim 500 \text{ eV}$; and an energy confinement time $\tau_E \hat{U} \hat{J}$ ms. (*M.G. Shats, H. Punzmann, K. Nagasaki, H.B. Smith*)

Remote Data Access

Experimental Java based remote viewers for the H-1NF magnetic field and power supply data were developed. Initial results indicate that the processing load can be successfully moved from the H-1NF server computer to a client PC. Work continues on a more comprehensive Java viewer combining the above with a local Java MDSPlus viewer from the University of Padua, Italy. Remote access using "Virtual Network Computer (VNC)" remote "virtual desktop" software has proven very useful for collaborators and facility users at remote sites. (*B.D. Blackwell, D. Price*)

H-1NF Data System

The MDSPlus data system, jointly developed by several international plasma fusion laboratories was implemented as the main H-1NF database during a visit by Thomas Fredian from MIT. 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 lossless data compression, and a convenient graphical interface. About two gigabytes of data in 2,000 pulses have been taken this year in tests, power tests and plasma pulses. (*B.D. Blackwell, J. Howard*)

Visualisation of Magnetic Design of Plasma Fusion Devices

An object oriented vacuum magnetic field line tracing code with real time stereoscopic display of field lines and conductor elements was implemented this year. Using a model of the heliac H-1NF, comprising 5000 finite filament elements, a computational step rate of 23,000 steps/second was achieved integrating along the magnetic field lines, with a 3D cubic spline array size of 64 MB, while maintaining a stereo display refresh rate of 30 frames/second on a personal computer. (*B.D. Blackwell, A. Searle*)

Other Activities

Exchanges with PRL's overseas collaborative partners in Japan and the USA continued during the year. Dr K. Nagasaki from Kyoto University, Japan, spent the period September 1998 to March 1999 in the Laboratory to continue his work with the H- 1NF electron cyclotron heating group. Professor K. Toi and Dr K. Kawahata from the National Institute for Fusion Science (NIFS) made visits in February and March respectively. Professor Toi worked with PRL on improved plasma confinement and Dr Kawahata on plasma diagnostic development. Dr T. Watari, also from NIFS, visited PRL in February to collaborate on the H-1NF ion cyclotron resonance heating of plasma. Dr Howard visited NIFS to install and test MOSS spectrometers on the Large Helical Device (LHD) fusion experiment.

Professor J. Harris continued to serve on the Stellarator Physics Advisory Committee at the Princeton Plasma Physics Laboratory in the United States.

Plasma Diagnostic Systems

Interferometry

The swept frequency 2 mm interferometer is being upgraded to provide four spatially distinct probing chords for the measurement of the plasma electron density profile. This instrument measures the line-of-sight integrated electron number density in the H-1NF plasma and is of crucial importance to machine operation. The new system will use temporal frequency multiplexing techniques to halve the number of detectors. The far-infrared scanning interferometer has also been successfully modified to operate at longer wavelengths (743 microns) in order to give greater sensitivity to low density plasmas produced during ECRH plasma generation. (*J. Howard*)

Diagnostics for Fluctuation Studies

Several new diagnostics devices have been set up on H-1NF to study plasma instabilities and turbulence. These are based on microwave scattering, and consist of electrostatic and magnetic probes and a twenty-channel correlation spectroscopy detector.

The microwave scattering diagnostic is based on a four-channel super-heterodyne detection system that measures the microwave power scattered from plasma density fluctuations. A microwave power of about 50 mW at frequency 132 GHz is scattered over a range of angles determined by the wave number of the plasma density fluctuations. This scattered power is collected by four quasi-optical antennas placed inside the vacuum tank of H-1NF. The diagnostic measures the frequency spectra and the wavelength content of the plasma turbulence as well as the propagation direction of the fluctuations in the plasma. The system has been modified in 1999 to improve its spatial resolution to about 0.2 of the minor plasma radius for all channels. http://rsphysse.anu.edu.au/~wms112/mscat

The correlation spectroscopy detector complements the microwave scattering by monitoring a range of plasma turbulence wavelengths above ~1 cm. The system consists of two linear optical fibre arrays (10 channels each) which are imaged into the plasma from two orthogonal views. Fluctuations in the plasma density and electron temperature contribute to the fluctuations in the measured intensity of the spectral line emission. By cross-correlating chord-average line intensities it is possible in some cases to obtain spatially localised fluctuation intensity, frequency spectra and the fluctuation correlation lengths. (*M.G. Shats, W. Solomon, H. Punzmann, D.L. Rudakov*) http://rsphysse.anu.edu.au/~mgs112/html/corspec.htm

Spectroscopy

Most work this year has focussed on the development of advanced diagnostic instrumentation based on the Modulated Optical Solid State (MOSS) spectrometer. The instrument is a modulated fixed-delay polarization interferometer based on electro-optic birefringent components. It is used for polarization and Doppler spectroscopy of radiation emanating from the neutral atoms and ions present in the plasma. Apart from significant instrumental advantages over grating spectrometers, we have formally demonstrated that for line-integral measurements of extended sources (such as plasmas), the information yielded by time-domain instruments bears a particularly simple relationship to line integrals of the spectral moments. The latter can be inverted to obtain spatially resolved information about local distribution functions or other plasma parameters that influence the spectral line-shape.

We have used the interlude provided by the H-1NF power supply upgrade to develop and install a number of new diagnostic tools based on MOSS technology. This program is summarized below:

• Installation of a rotatable array of 55 lens-coupled optical fibres for tomography of the ion flow and temperature profiles in the H-1NF. The system will be commissioned by the end of the year.

http://rsphysse.anu.edu.au/~jnh112/MOSS/TOMOSS.html

• Construction and characterisation of a 16 channel MOSS camera for studies of plasma transport using heating power perturbation techniques. http://rsphysse.anu.edu.au/~jnh112/MOSS/camera.html

• Development of a LabVIEW driver for PCI-MIO-16E-4 data acquisition card, PC-based operation of a single channel MOSS system. This system is being tested on the LHD stellarator at the National Institute for Fusion Science in Japan in December.

• Theory, simulation and construction of multiple fixed delay Spread-spectrum Optical Fourier Transform spectrometer (SOFT), an extension of the MOSS concept. This system, which has been granted a provisional patent, allows time-resolved highresolution study of spectral lineshape details. The information is encoded on a number of discrete carriers (channels) in the temporal frequency domain.

http://rsphysse.anu.edu.au/~jnh112/MOSS/SOFT.html

• In-vacuum installation of a number of fixed lens-coupled optical fibres for MOSS/SOFT study of ion distribution functions and plasma toroidal flows. (J. Howard, F. Glass, C. Michael, A. Cheetham, A. Last, J. Wach, M. Blacksell, R. Davies)

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 summarized below. The Group is currently planning 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 will run for the first time in 2000.

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]; *M. Shats*)

Plasma Theory (Flinders University)

A resistive magnetohydrodymanic (MHD) stability and spectral code, SPECTOR-3D, is being developed for 3D helical configurations to be applicable to stellarators and, in particular, to the H-1NF. The collaboration began this year and will be funded by an AINSE travel grant in 2000. (*R. Storer [FU]; H.J. Gardner*)

Soft X-ray Measurement System (University of Canberra)

Soft X-ray systems for measuring plasma pressure, the effects of impurities and the electron temperature are currently being installed. Assoc. Professor Cheetham from the University of Canberra has been working at the facility for six months as a Visiting Fellow while on study leave. A 16 channel single chip X-ray detector is being installed. Viewing the plasma through a beryllium covered slit, the system will allow up to 16 chord integrated measurements of the X-ray flux across the plasma. (*B.D. Blackwell; A.D. Cheetham [UC]*)

Laser Induced Fluorescence (University of Sydney)

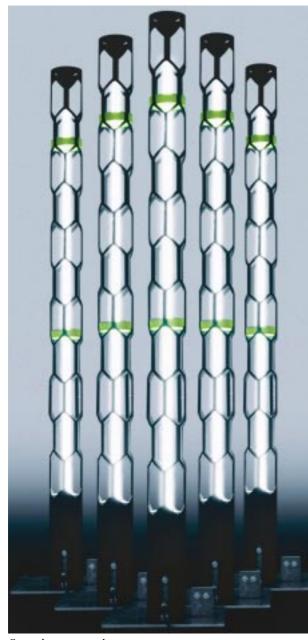
A laser induced fluorescence system has been purchased from RIEF funds for measurement of electric fields and particle velocity distribution functions in the H-1NF plasma. An Australian Research Council Large Grant application has been successful and will support a three-year postdoctoral position to implement and use this system. The position is about to be advertised. This work is being coordinated by the University of Sydney. (*J. Howard; B.W. James [U. Sydney]*)

Fibre Sensors (University of New England)

The University of New England is involved in developing, constructing and installing novel optical fibre sensors and bolometers for electric field and thermal measurements in the edge and body of the H-1NF plasma. The insulating nature and immunity to high voltage and electromagnetic noise of these devices makes them particularly attractive for plasma work. They are providing new information on H-1NF that is not readily available from more conventional probes. (J. Howard, B.D. Blackwell, J.H. Harris; V. Everett, G.B. Scelsi, G.A. Woolsey [UNE])

Plasma Antennas

In January 1998, the Plasma Research Laboratory won a contract offered for tender by the Defence Science and Technology Organisation (DSTO) to investigate the feasibility of plasma antennas as low radar cross-section radiating elements. This first stage of the contract was successfully completed last year. The second stage of the contract to develop a concept demonstrator plasma antenna was successfully completed in November this year. Four ANU Honours engineering students



Second prototype plasma antennae

have now completed their projects on the plasma antenna, and a relevant publication has appeared in Applied Physics Letters.

In November, a SPIRT grant was won by the Laboratory with CEA Technologies (Canberra) and Neolite Neon (Sydney) to develop a commercial plasma antenna for ship-borne radar and communications. The grant will be used to fund a PhD scholar to work on the project. An invited paper on the plasma antenna was presented at the 41st American Physical Society Conference held in Seattle, Washington in November. (*G.G. Borg, J.H. Harris, D.G. Miljak*)

http://rsphysse.anu.edu.au/~ggb112

Space Plasma and Plasma Processing Group

The SP³ 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 germanosilicate 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; F. Ladouceur, J.D. Love[OSC]*)

Breakdown in Continuous and Pulsed Radiofrequency Plasmas

Breakdown in a parallel plate rf system has been studied using experimental, computational and analytic techniques in the 1-500 mTorr pressure (p) range and for electrode separation (d) of 2-20 cm. A Particle-In-Cell (PIC) simulation has been used to investigate the effect of the secondary emission coefficient on the rf breakdown curve, particularly at low pd values. A zerodimensional global (volume averaged) model has also been developed to compare with experimental and simulated measurements of breakdown.

Development of these experimental and computational studies has also been made for much lower pressures where additional processes involving metastable atoms and ions have to be taken into account when modelling the breakdown. (C. Charles, H. Smith)

Plasma Etching with SF₆

The plasma and gas phase species in a SF₆ plasma have been measured for pressures between 0.3 and 7.5 mTorr in a helicon reactor. Two different regimes have been observed. At low power for all pressures the ionization takes place in the diffusion chamber due to capacitive coupling, the main ionic species being SF³⁺. At high power, the plasma is highly dissociated with the main ionic species being F⁺ and S⁺ created in the source and diffusing into the diffusion chamber. The dissociation mode depends both on the gas flow and pressure. These studies are very important for the etching of silicon based semiconductors where SF₆ is a common etch gas. *(T.E. Sheridan, P. Chabert, R.W. Boswell)*

Helicon Assisted Reactive Evaporation (HARE)

Helicon Assisted Reactive Evaporation (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, S. Hatch*)

Large Volume Helicon Source Experiments

A series of experiments were conducted to launch Trivelpiece-Gould modes in a 9 cm radius, 50 cm length helicon source. Waves were excited using a small electrostatically coupled auxiliary antenna, scanning frequencies from 1 to 30 MHz. Maps of the wave amplitude and phase were made within the source by scanning the position of a dog-leg electrostatic probe and bdot probe. At low densities, the amplitude maxima corresponding to the group velocity resonance cone angle were found to decay as the distance from the antenna was increased with some indications of reflections when the resonance cone peaks intersected the radial boundary of the source. The observed radiation pattern in most cases was consistent with that of a point source in an unbounded plasma. No global eigenmode resonances were found as predicted theoretically by a number of authors. As the density was increased, the amplitude maximum along the resonance cone angle became less distinct as the wave became more electromagnetic (helicon-like). (A.W. Degeling, R.W. Boswell, G.G. Borg)

Helicon Mode Transitions

The helicon wave-heated plasma can produce a very high-density plasma for low gas pressures and a weak magnetic field configuration. Three categories of plasma heating exist for this system: capacitive (E-), inductive (H-), and helicon wave driven (W-) modes. The development of a particular mode depends on the external parameters such as pressure, magnetic field, and rf power. Much work has gone into understanding the transitions between these modes.

The mode transitions have been primarily studied using electrical measurements. We have experimentally observed and characterised five distinct discharge modes in an axially-short, weakly-magnetised helicon discharge. The helicon wave vectors were shown to correspond to cavity-mode resonances of the plasma-filled vessel. Increasing the electron collisionality by raising the neutral gas pressure was found to decrease the Q (quality factor) of the resonances. The first unambiguous evidence of a propagating m = -1 mode (long predicted by theory) has now been observed. (*K.K. Chi, R.W. Boswell, T.E. Sheridan*)

Retarding Field Energy Analyser and Multiple Retarding Field Energy Analyser

The helicon system "Chi Kung" comprises a 15 cm diameter pyrex source tube 30 cm long attached to a 30 cm diameter, 30 cm long aluminium diffusion chamber and 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 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.

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 visualization 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 multidimensional data and often this is difficult within the confines of a two-dimensional screen. The WEDGE virtual reality theatre was developed in collaboration with the ANU Supercomputer Facility, and opened in April 1998. It is the first walk-in virtual reality theatre in Australia and the first in the world to be based on PC technology.

The WEDGE has two large screens at right angles on which the data images are back projected. A powerful PC with fast graphics capability is used to generate the two images in stereo for each screen and the resultant 3-d image seems to float in the space between the screens when viewed with special liquid crystal display glasses. The WEDGE has been used to model the H-1NF Heliac and collaborative efforts with groups in Biology, Astronomy, Earth Sciences and Psychology are being developed. Further information about the WEDGE can be found at the web address: http://WEDGE.anu.edu.au/

A similar system to the WEDGE, but using only a single screen, is located in the H-1NF control room. The system is set up to display video and computer-generated slide presentations, as well as 3-D images, and will be used for talks and outreach programs as well as for research purposes. (*R.W. Boswell, H.J. Gardner, R.P. Hawkins*)

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C. Costa

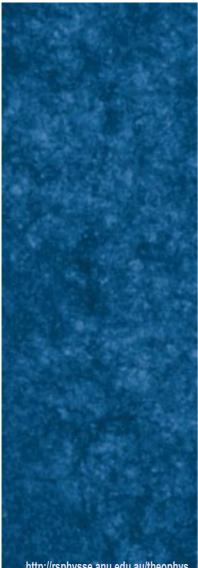
Departmental Administrator H.P. Hawes, BA

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Research Accomplishments



Professor Robert Dewar - Head of Theoretical Physics



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

Theoretical Physics

The Department of Theoretical Physics performs research at the highest international levels in selected areas of theoretical, mathematical and computational physics in partnership with experimental groups working in related areas of physics. Through the Centre for Theoretical Physics it fosters multidisciplinary research by organising topical research workshops, and plays an important national role in postgraduate education by holding annual graduatelevel Physics Summer Schools.

Research Summary

A new trend in physics known as the Complex Systems approach is characterised by the idea that the fundamental goal of physics is to build a rigorous intellectual framework that leads to a quantitative understanding of nature on all scales, by working upwards from the laws of nature at the microscopic scale. This view of physics contrasts with, but is complementary to, the traditional reductionist approach, in which it is assumed that ultimately nature will be understood if we study matter at ever finer scales

Fundamental aspects of physics on all scales are covered in the research interests of the Department. Although the boundaries can (and, according to the Complex Systems paradigm, should) overlap, for convenience the research is reported here under the headings of Microscale Physics (from the atomic scale downwards), Mesoscale Physics (assemblies of atoms into lattices and small structures, including mesoscopic systems, where quantum mechanics is 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's research strength in areas relevant to practical applications has been recognised this year through the award of two grants from the Department of Industry, Science and Resources (DISR) under its Industrial Research Alliances Program (IRAP): \$14,000 for an international workshop on High Performance Computing and Advanced Visualisation in Plasma Physics Research to Professor Dewar, and \$20,000 to Dr Gulacsi to assist international collaboration on Impurity Effects in Mesoscopic Systems.

The Department is host to The Australian National University Centre for Theoretical Physics, which fosters cross-disciplinary research and graduate education through annual summer schools and topical workshops (see page 89). This year's successful summer school on Quantum and Classical Chaos was organised by department members Dr S. Y. Kun and Dr M. Gulacsi, and covered a wide range of interesting topics, from nuclear physics to modes in microwave cavities.

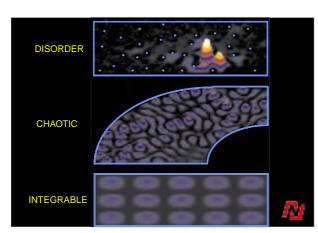
Mesoscale Physics

Condensed Matter Physics

Electron Correlations in Solids

Strong electronic correlations seem to influence the physical properties of solids, resulting in peculiar anomalies. Using the Hubbard model we have studied the metalinsulator transition, various aspects of the normal state of high- T_c superconductors, and the effect of substitutional impurities for Cu within the CuO planes of the high- T_c materials. By doping with non-magnetic impurities such as zinc at copper sites, we have obtained information on the local moments near impurities. The relevance of this model on copper-site substitution in high- T_c materials is being examined, using the experimental results of the Wollongong group. (M.P. Das)

Ab initio calculations of excited states of solids have gained a lot of interest due to the advent of high-performance computers making such calculations feasible. Experimentally, a wealth of information about such states can be obtained by means of



Measured microwave intensity distributions for three "quantum billiard" experiments. (Courtesy Professor S. Sridhar, invited lecturer, Summer School in Quantum and Classical Chaos, 1999)

ionisation spectroscopy after removing an electron from the correlated electron ensemble in a solid. A suitable method for studying the effect of many-electron correlations on the excited-state properties of extended systems is the Green function method. The simplest approximation for the self-energy beyond the Hartree-Fock approximation that takes into account screening is the so-called GW approximation (Green/screened Coulomb interaction), which can incorporate a realistic crystalline structure. Further vertex corrections 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 in AMPL. (A.S. Kheifets; F. Aryasetiawan [Lund])

In theoretical physics unitary transformations are used to obtain a deeper insight into physical phenomena, the aim being to transform the Hamiltonian for a system so as to reveal the appropriate independent subsystems. A method has been developed by which a unitary transformation can be performed up to infinite order. This exact method was successfully used for three-dimensional interacting (non-integrable) quantum field theory models of Anderson type and two- and/or three-band Hubbard models. (*M. Gulacsi, R. Chan*)

A new Density Matrix Renormalisation Group (DMRG) method has been developed which conserves all the quantum numbers, most importantly the total spin. This new method was successfully applied to several strongly correlated electron systems, in particular to the one-dimensional Kondo lattice model where the exact phase boundaries and the extent of the Fermi surface were determined. This clarified the controversy over the extent of the Fermi surface, the central issue for much research in impurity models. This new DMRG method was applied to several other models in collaboration with co-workers in Stockholm, Los Alamos and Stuttgart. (*M. Gulacsi, I. McCulloch*)

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 non-equilibrium fluctuations in metallic mesoscopic systems, accounting for the dominant Fermi liquid behaviour of the electrons. The Pauli exclusion principle determines electronic properties of a metal near equilibrium from the microscopic level to the bulk. We have studied within a microscopic kinetic approach how degeneracy determines non-equilibrium current noise over a wide range of length scales, even at high fields, raising some important issues on the currently used semiclassical diffusive theory for the shot noise, thermal noise and their crossover. (*M.P. Das; F. Green [CSIRO]*)

Density Functional Theory of Super-phenomena

Experience shows that, at 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 superphenomena (superconductivity and superfluidity). In the realm of density functional theory we are studying the occurrence of Fermi and Bose condensates in appropriate situations as fundamental processes. Our aim has been to obtain a pairing potential that sustains an order parameter due to broken symmetry. (*M.P. Das*)

Resonant Solitons in Semiconductors

Numerical work on the dynamics of resonant solitons in the excitonic spectral region of semiconductors has been continued with a focus on potential applications in ultrafast optical signal processing. In addition to recent results that demonstrated the possibility of highly efficient, low-latency, optical switching in a semiconductor nonlinear directional coupler (NLDC) in the Tbit/s regime, the operation of a variety of resonant soliton logic gates has been investigated. Using the resonant soliton logic gates, the feasibility of optical packet processing in time-division-multiplexed (TDM) networks at Tbit/s bit rates has been demonstrated numerically. The operation of key components in TDM receiver nodes with functionalities such as packet address recognition, buffering, and packet routing has been modelled. (*I. Talanina [supported by the US Air Force Office of Scientific Research]*)

Bose-Einstein Condensation

Recent experiments on ultracold dilute vapours of hydrogen and alkali atoms in electromagnetic traps reveal Bose–Einstein condensation (BEC) in the nano-Kelvin range of temperatures. This will be the topic of the Centre for Theoretical Physics Summer School being organised for January 2000.

The Gross-Pitaevskii formalism allows two- and three-body interactions to be explicitly included. It is found that, for low-dimensional systems, interplay between attractive and repulsive interactions among the atoms can lead to the formation of the BEC. The kinematics of Bose–Einstein condensates in a cylindrical geometry has been studied using a time-dependent, fully three-dimensional numerical code. Numerical results show that periodic, aperiodic or quasi-chaotic behaviours in the condensate wavefunction can be observed depending on the number of trapped atoms. (*M.P. Das, N. Akhmediev [OSC], M. Gulacsi, J.L.V. Lewandowski*)

Mathematical Physics

Statistical Mechanics and Related Field Theories

The field of solvable models in statistical mechanics has ramifications in many areas, such as integrable models, quantum field theory, random matrix models, knot theory, quantum groups, and various problems in combinatorics. The chiral Potts model continues to present fascinating challenges: in particular two expressions for the free energy were obtained in 1988 and until now it has not been at all obvious that they agree. This problem has now been resolved: it has been explicitly shown that they are completely equivalent. (*R.J. Baxter*)

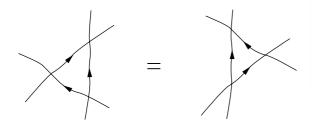
The Zamolodchikov model is a solvable three-dimensional model. It shares some intriguing symmetries with the simple "free-fermion" three-dimensional model, which makes one speculate that the methods of the latter may apply to the former. These ideas are easy to test for the two-layer case, this has been done and a number of simple and indicative properties have been observed. (*R.J. Baxter, V.V. Bazhanov*)

Various Yang-Baxter integrability structures in quantum field theory were studied. In particular, a new and fascinating connection between the spectral properties of Baxter's Q operators in conformal field theory and the spectral properties of the one-dimensional Schrödinger equation has been established. Using this connection, it has been possible to prove the strong-weak barrier duality relation for the nonlinear mobility related to the impurity transport in a nonequilibrium Luttinger liquid. (V.V. Bazhanov, S.L. Lukyanov, A.B. Zamolodchikov)

The systematic analysis of the finite-temperature properties of the Luttinger liquids was continued, using thermodynamic Betheansatz equations in conjunction with finite-temperature non-Abelian Bosonisation techniques. The complete form of the momentum distribution function at finite temperatures was calculated for all delta-function interacting models. (*M. Gulacsi, G. Bowen*)

The functional relations for the commuting transfer matrices for models with higher symmetries were studied from an algebraic point of view. A quantum Boussinesq theory has been developed that describes the integrability structure of the conformal field theory with extended *W*-symmetry. (*V.V. Bazhanov, A.N. Hibberd, S. Khoroshkin*)

It has recently been shown that there is only one measure of uncertainty or spread for classical and quantum ensembles that satisfies basic geometric notions. This provides a new geometric interpretation of entropy, and is applicable to derivations in quantum information, statistical mechanics, uncertainty relations and dynamical processes. (*M.J.W. Hall*)



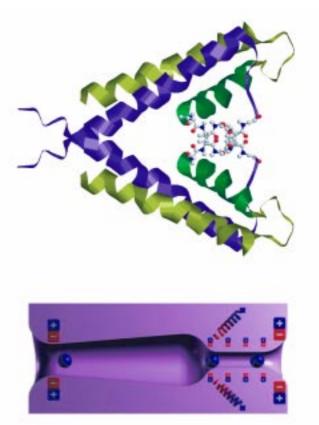
Graph-theory representation of the famous Yang-Baxter relation used in finding solvable models

Biophysics

Ion Channels in Biological Membranes

The work on ionic channels of biological membranes continued on two fronts: one was establishing Brownian dynamics (BD) as the method of choice in channel current calculations, and the other was providing a comprehensive description of the potassium channel, whose molecular structure was recently discovered. Continuum approaches such as solving Poisson-Nernst-Planck (PNP) equations for channel currents and Poisson-Boltzmann (PB) equations for electric potentials are still regularly used in models of ion channels. On the basis of channel sizes and numbers of ions involved, it is difficult to justify the application of these mean field methods in the channel problems. We used Brownian dynamics simulations to check the validity of the PNP and PB theories in simple cylindrical and spherical geometries with varying radii. Both theories are found to strongly overestimate the shielding effect on an ion when the boundaries are within 1-2 Debye lengths, and thus neglect the effect of the induced surface charges on channel walls. Since, in a typical channel environment, the Debye length is about 10 Å and the channel radius is much smaller than that, we conclude that the continuum theories are not reliable for use in studies of ion channels. (S.H. Chung [Chemistry, The Faculties], B. Corry, S. Kuyucak)

Molecular Dynamics (MD) simulations can play an important role in channel studies by providing realistic values for the various



The structure of the potassium channel found from X-ray diffraction (top) and the simplified model used in Brownian dynamics studies (bottom). The selectivity filter is shown in atomic detail while the outer and inner helices are indicated with ribbons. The blue balls show the positions of 3 potassium ions at the beginning of a typical conduction event.

parameters used in more phenomenological approaches (e.g. diffusion coefficient, dielectric constant, etc.). For this purpose, we have carried out MD simulations of ions in water confined in a cylindrical boundary with varying radii. The boundary is also varied from that of a passive hard wall to an active one lined up with dipolar molecules. The results show that the diffusion coefficient of ions is sensitive to the correlation between the channel radius and the hydration radius, as well as the type of boundary one uses. Another application of the MD is the explanation of the selectivity of ion channels. The molecular structure of the potassium channel has recently been determined from X-ray diffraction. This channel conducts K but not Na ions. Using the given structure information in the MD simulations, we were able to show that the selectivity arises because the carbonyl groups in the selectivity filter can successfully solvate K but not Na, which has a considerably smaller radius. As a result, Na ions encounter a large energy barrier (~20 x thermal energy), limiting their permeation across the channel. (T.W. Allen, S.H. Chung [Chemistry, The Faculties], S. Kuyucak)

Microscale Physics

Particle Physics and Quantum Field Theory

Two projects on the application of the Dyson-Schwinger equations to quantum electrodynamics have been completed. Firstly, the supersymmetric extensions of quantum electrodynamics in three and four space-time dimensions were investigated. The most promising theories that attempt to unify the fundamental forces of nature are, by and large, supersymmetric. However, because of their complexity, extracting the physical consequences of supersymmetric models is a formidable task. Our research has demonstrated that the Dyson-Schwinger equation approach can be successfully applied to non-perturbative studies of supersymmetric field theory. Secondly, we have exploited the Dyson-Schwinger equations and their transformation properties under local gauge transformations to obtain exact results concerning the solutions of three-dimensional quantum electrodynamics in the limit in which virtual electron-positron pairs are suppressed. In addition, work on the Bethe-Salpeter model of the observed light pseudoscalar and vector mesons has been shown to successfully explain the mass of the $\hat{\rho}$ meson. (C.J. Burden, M. Walker, P. Tjiang; M.A. Pichowsky [Indiana U.])

Nuclear Theory

The robustness of the conjectured correlation between the gfactor ratios in the ground and gamma bands, and the corresponding E2/M1 mixing ratios in the proton-neutron interacting boson model (IBM) has been investigated. This correlation was shown to be dependent on the choice of the Hamiltonian and can be transgressed when the parameters are chosen appropriately. The recent M1 data in ¹⁶⁸Er, which does not exhibit such a correlation, are analysed in the light of these results. The IBM can accommodate the new M1 data by including parameters that are not usually used in the model. As there are inconsistencies in the M1 data, their remeasurement in ¹⁶⁸Er is desirable before reaching a definite conclusion on whether an extension of the standard parameter set in the IBM is required. *(S. Kuyucak; B.R. Barrett [Arizona])* Shape-phase transitions in mixed parity boson systems have been studied using mean-field theory. Without parity projection, shape transitions in mixed parity systems are very similar to those in unique parity systems, both requiring a finite interaction strength for the onset of deformation. The shape-phase diagram in mixed parity systems, however, changes significantly after parity projection, with the critical point for the onset of octupole deformation moving to zero strength. Shape transitions in the Lipkin model exhibit the same features, indicating that this is a direct consequence of parity projection in finite, mixed parity systems independent of the nature of interacting particles. *(S. Kuyucak)*

Work on a project to analyse the available π^{\pm} p scattering data up to a pion laboratory kinetic energy of 100 MeV has made good progress. While the π^{\pm} p elastic scattering data can be satisfactorily fitted, there is evidence from the π^{-} p charge exchange scattering data for violation of isospin symmetry. (W.S. Woolcock; G.C. Oades [Aarhus]; G. Rasche, E. Matsinos, A. Gashi [Zürich])

Theoretical studies of the ${}^{9}Be(p, \alpha){}^{6}Li$ and ${}^{9}Be(p, d){}^{8}Be$ reaction data has continued to accommodate new experimental results. *(F.C. Barker, Y. Kondo [Kyoto Women's University]).*

The effect on the low-energy ⁷Be(p, γ)⁸Be S factor of a broad 2⁻ level in ⁸B at 3 MeV, as had been observed in ⁷Be+p elastic scattering, has been studied, and it is concluded that the level must have a width ≥4 MeV. (*F.C. Barker; A.M. Mukhamedzhanov* [*Texas A&M U.*])

Using the distorted wave impulse approximation, the inelastic scattering cross section and polarization for the ${}^{12}C(p, p'){}^{12}C^*$ (2⁺, 3⁻ and 1⁺) reactions have been calculated for antiproton energies of 46.8 and 179.7 MeV. The calculations are in good agreement with the available data. (*B.A. Robson; Zhang Yu-Shun [Inst. High Energy Physics, Academia Sinica]*)

It is known that in the spontaneous fission of a heavy nucleus many more neutrons are emitted than predicted by the Bohr-Wheeler statistical model. One reason often advanced to explain this phenomenon is nuclear friction, which slows down the deformation of the nucleus so that the fission time becomes longer. Work has commenced to develop the usual classical approach employing a Fokker-Planck equation to investigate in more detail the effect of friction on spontaneous fission. (B.A. Robson; G.D. Dang [U. Paris-Sud])

Exotic atomic systems such as singly-charged heavy ions like uranium-91⁺ are valuable testing grounds for quantum electrodynamics and relativistic quantum theory. Previous work using the dipole approximation for such 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. This work has been extended to calculate the transition probabilities without making the dipole approximation and also to calculate the so-called "forbidden" components. The results confirm that the eight-component and Dirac theories predict different transition probabilities for the components of the Balmer- α and Lyman- α lines. (*B.A. Robson, S.H. Sutanto*)

Correlations and Decoherence in Quantum Systems

Deterministic randomness has been obtained within the theory of spontaneous correlations and slow decoherence in complex microscopic and mesoscopic systems (CMMS). The experimental test of this novel phenomenon has recently been performed in a collaborative venture between Chinese scientists and ANU. The analysis of the data is in progress. (*S.Yu. Kun; Wang Qi et al. [Inst. Modern Physics, Lanzhou, China]; Li Songlin et al. [Inst. Atomic Energy, Beijing]*)

It has been shown for the first time that the decoherence sets up a new energy scale for quantum many-body CMMS. This scale is analogous to the Thouless energy in disordered systems. Beyond this new scale, the random-matrix theory of quantum many-body systems ceases to apply. This leads to a number of novel microscopic and mesoscopic phenomena, which are currently being studied. (*S.Yu. Kun; H.A. Weidenmüller [Max Planck Institute for Nuclear Physics, Heidelberg]*)

A common manifestation of the violation of random-matrix theory in microscopic and mesoscopic systems is oscillating structures of the energy autocorrelation functions for heavycomplex quantum collisions and coherent electron transport in quantum dots. The theory of spontaneous correlations and slow decoherence has been applied to the analysis of these oscillating patterns in CMMS. An indication for the excitation of highly excited many-body Schrödinger-cat states has been found in heavy-ion elastic and inelastic scattering. (S.Yu. Kun, B.A. Robson; A.V. Vagov [UWA]; O.K. Vorov [Sao Paulo])

Quantum carpets are patterned structures in the space-time probability distributions of one-dimensional quantum systems, first discovered in 1995. Work has continued an a new approach for predicting these structures for the infinite-square-well potential, based on a representation of the probability density P(x,t) as a discrete sum of travelling waves. (*M.J. Hall, M. Reineker; W. Schleich [Ulm]*)

Macroscale Physics

Nonlinear Dynamical Systems

Dynamical systems theory is the body of mathematics concerned

with the global characterisation of the time evolution of a finite or infinite set of variables. Often the long-time behaviour of an infinite-dimensional system can be described by a finite set of "master" variables because, after an initial transient, most of the variables (the "slaves") relax so as to follow the master variables adiabatically. The identification of such master variables and the determination of their dynamics thus provide a methodology for the understanding of complex systems. A review of dynamical systems theory in this context was published this year. (*R.L. Dewar*)

An important tool for global analysis is *singularity theory*. The mathematics of

singularity theory is profound and rather difficult, so novel visual interpretations of singularities are being developed. These have more than heuristic value: visualisation of singular surfaces is a powerful new aid for the design and control of dynamical systems generally.

The analysis of confinement transitions in the H-1NF heliac is an application of singularity theory currently being developed (see Plasma Theory section). Another application, with important safety implications, has been to the nonlinear dynamics of cellulose thermal decomposition. It was shown that a commonly used fire-retarding treatment can actually increase flammability in situations of restricted heat transfer, such as cellulose insulation, furnishings and bedding, and bagasse stockpiles. (*R. Ball*)

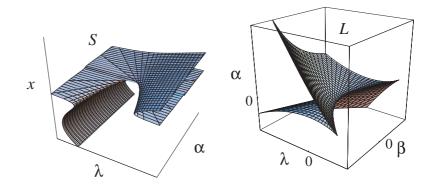
A book for honours undergraduates or graduate students is being written which will give an overview of mathematics, not only for mathematicians who wish to know something outside their own speciality, but also for physicists, engineers, teachers and others with a serious interest in mathematics. (W.A. Coppel)

Plasma Theory

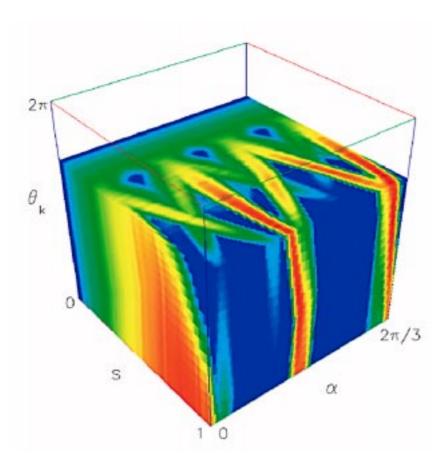
Plasma confinement in toroidal geometry is determined not only by collisional transport but by complex nonlinear interactions involving sheared background flows and low-frequency collective modes (drift waves). At higher pressures, deformation of the equilibrium magnetic field, and pressure-driven instabilities (ballooning modes), are also important. Work on aspects of these phenomena is carried out in the plasma theory group, with a particular interest being to predict or explain behaviour in the H-1NF heliac in the Plasma Research Laboratory.

An overall understanding of the novel characteristics of local ballooning mode behaviour in low-magnetic-shear, low-aspectratio stellarators such as H-1NF has been developed using the concept of Anderson localisation due to the quasi-periodic dependence of equilibrium parameters along a magnetic field line. This leads to strong field-line dependence of the growth rate. *(P. Cuthbert, R.L. Dewar)*

Work has begun on modelling the discontinuous dependence of



S is a solution manifold of a nonlinear dynamical system that has a pitchfork bifurcation as an organizing centre. Singular points on S unfold to an invariant manifold L around the pitchfork at (0,0,0).



Parametric dependence of local ballooning mode growth rate in H-1NF. The variables s and α specify the field line and θ_k determines the direction of the wave vector

confinement properties observed in H-1NF as control parameters are varied, by adapting low-dimensional dynamical systems models developed for tokamaks and applying singularity theory. Preliminary results indicating that the Low to High (L-H) confinement transition is intrinsically oscillatory, potentially hysteretic, and controlled by three parameters. *(R. Ball, R.L. Dewar)*

The behaviour of magnetic islands at fusion-relevant plasma pressures is of much interest for low-shear stellarators such as H-1NF. 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 the 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. (H.J. Gardner, S.S. Lloyd)

The development of a fully three-dimensional resistive magnetohydrodynamics (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; R.G. Storer* [*Flinders*])

A method for calculating the transit-time dependence of the heating of particles by waves (Fermi acceleration) has been developed for particles chaotically confined by cusp fields. (*R.L. Dewar; C.I. Ciubotariu [Lethbridge]*)

The effect of a finite radial wavenumber on collisional drift waves in the geometry of the toroidal heliac H1-NF has been studied. It was found that a vanishing radial wavenumber yields the fastest linear growth rate. (J.L.V. Lewandowski, R. Ellem)

The radial structure of electron drift waves has been calculated in toroidal geometry. Analytical calculations show that the radial extent (and associated anomalous transport) of the toroidal drift wave depends nonlinearly on the shear and curvature of the safety factor profile. For typical medium-sized tokamak edge plasmas the calculated anomalous transport was found to be up to one order of magnitude larger than previous estimates. (J.L.V. Lewandowski)

Cosmology

The Isotropic Singularities project is an examination of a subclass of Big Bang type initial cosmological singularities, which have an associated conformal structure that is regular. During this year work has centred round discovering a characterising feature for perfect-fluid space-times that admit an isotropic singularity. It has been shown that, contrary to expectations in the literature, the Weyl tensor cannot be a characterising feature. Significant progress on this problem is currently being made using new approaches. (G. Ericksson, S.M. Scott)

Collaborative work has continued on a possible explanation for the observed non-uniform distribution of matter in the universe based on the idea that the present universe was formed by the fragmentation of macroscopic superstrings. (*L.J. Tassie; P. Brosche [Bonn]*)

Visualisation

The WEDGE, which was developed in collaboration with Professor R.W. Boswell, Plasma Research Laboratory and Mr Drew Whitehouse of the ANU Supercomputer Facility, is the first walkin virtual reality theatre in Australia. It shows great promise for various applications in scientific visualisation. (*H.J. Gardner*)

The WEDGE has featured in much outreach activity for the ANU including the Australian Science Festival. Commercialisation activities have resulted in a WEDGE installation at the Powerhouse Museum in Sydney as part of their "Universal Machine" installation and other negotiations are continuing. A version of the WEDGE is being built to display real time stereo video from remote sites as part of a robotic control centre. Further information about the WEDGE can be found at the web address http://wedge.anu.edu.au/

During the year a portable version of the WEDGE was built and displayed at an international workshop on *High Performance Computing and Advanced Visualisation in Plasma Physics Research* at Magnetic Island, Queensland, in July. In October it featured at the launch of the Australian Partnership for Advanced Computation at Parliament House, Canberra. Interactive three-dimensional graphics has great potential in such applications as understanding chaos in four-dimensional symplectic maps, analysis of singularities in bifurcation theory, general relativity etc. Efforts are under way to develop visualisations in these areas using both high-level languages such as IDL and Mathematica and using the lower-level OpenGL libraries. (*R.L. Dewar, R. Ball, H.J. Gardner, A. Searle, S.M. Scott*)

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A.S. Kheifets, MSc PhD St Petersburg (jointly with AMPL)

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