Applied Mathematics

Professor Stephen Hyde
- Head of Applied Mathematics

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

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

Research Summary

This year marks the 65th birthday of our Founding Professor, Barry Ninham. As a result, Barry formally retired at the end of the year. His retirement is a formal one only, and the Department hopes that he will be with us for many years yet. Such occasions demand politeness, a nicety that makes it difficult to express the genuine depth of gratitude we owe Barry for so many years of dedication and belief in the department that he built. His sheer energy has forged a world-beating group over three decades. His style has indelibly marked the Department: we remain an informal, inquiring inter-disciplinary group, interested above all in the scientific questions that lie between the traditional disciplines. Barry remains active on many fronts; research continues here and in Europe. In addition, his commitments to UNESCO continue, where he is setting up an international network of institutes to study all aspects of water resources, a looming problem in many parts of the globe. The ANU will host one of those nodes; others are being set up in Scandinavia and elsewhere. Another of our most senior members, Professor Stjepan Marcelja has been appointed Director of the Rudjer Boskovic Institute in Zagreb. The appointment, leading an institution with over four hundred scientists, testifies to the highest international status of our group. We congratulate him, and hope to see him return to science here as often as possible.

This year signals the first formal entry into the national ARC grant scheme. The Department achieved 100% success in 2001, a record that we hope to match in the future. We are also one of three research centres (Applied Maths, CSIRO Forest Products and Chemical Engineering, Monash University) for the new government-funded Cooperative Research Centre for Functional Communication Surfaces, a university-industry centre distributed across the country to develop Australian paper and printing capabilities. Despite the difficulties besetting higher education in Australia, we maintain a healthy balance between pure and applied research.

To continue as a dynamic research group within the Institute of Advanced Studies, it is essential that we continue to forge new research paths, without forgetting our traditional strengths. Our interests are evolving each year, and they now include areas beyond traditional colloid science, such as self-assembly of inorganic precipitates, characterisation of ordered and random networks, the physics of paper products and transport of inks within paper, novel carbon materials and fluid transport in random porous media. Three research streams can now be discerned: one concerned with surface forces, a second with self-assembly and a third with complex real-world materials. The three remain linked by common interests and expertise, and Department members share common interests across the spectrum of applied mathematics research. The intimate mix of theory and experiment remains an essential aspect of our work, with the accretion of a substantial computational strand, aided by funding from the Australian Partnership for Advanced Computation. This year has seen a resurgence of surface forces efforts: real advances have been made in understanding of the hydrophobic interaction, specific ion effects and hydration/solvation forces. Pioneering Atomic Force Microscope (AFM) experiments have uncovered boundary slip in simple fluids at walls, a result that has generated much publicity. Real progress has been made in deciphering random structures from 2D images, as well as cataloguing 3D networks.

On a personal note, the Department extends its congratulations to Professor Stephen Hyde's father, B.G. Hyde, on the completion of his book, *David Wadsley's science*.

Surface Forces and Colloid Science

Observation of Capillary Forces in Vapours of Various Liquids

Forces between the fluorocarbon monolayer surfaces were measured under various vapour conditions with the interfacial gauge. The force profiles in vapours of ethanol or chloroform agree with the theory of capillary bridging by constant volume meniscus.

In vapours of perfluorohexane, the interaction form changed to the capillary force for the meniscus in equilibrium with the vapour. The condensate volumes and the relative vapour pressure were estimated by fitting the measured force curves with theoretical forms. (S. Ohnishi and V. Yaminsky)

Interaction of Surfaces or Macromolecules in Aqueous Solvent

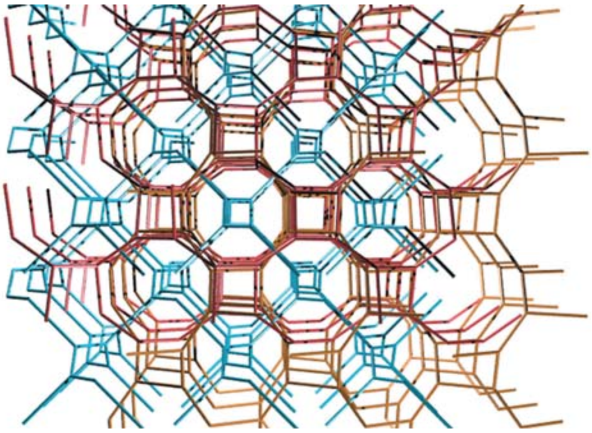
We continued with development of the method where electrostatic forces and potentials between surfaces or macromolecules in aqueous solutions are calculated using effective potentials between ions in water. The potentials are obtained from simulations of the full molecular model of an ionic solution.

In the next year we require further development, particularly in the simulation of particle-surface effective potentials. Eventually we can envisage many applications in the colloid and surface sciences as well as in the more complex field of predicting interaction and binding involving biological macromolecules. (S. Marcelja; A. P. Lyubartsev [Stockholm University, Sweden]; S.-J. Marrink [University of Groningen, The Netherlands])

Newtonian Fluid Slip along Walls

Accurate measurements of drainage forces between an approaching sphere and flat surface have revealed the presence of boundary slip in aqueous Newtonian solutions. The degree of slip has been characterised and is revealed to be dependent upon the shear rate and viscosity of the fluid. Hydrodynamic forces have also been utilised as a means to accurately determine the spring constant of colloid probes (very fine Atomic Force Microscope cantilever springs with a sphere placed at the end). This method is convenient, accurate and highly suitable for colloid probes used in surface force measurement. A technique has been developed to further characterise colloid probes by conveniently determining the radius of curvature of the colloid probe in the interaction region and analysis of the surface features of the colloid probe. This involves 'reverse imaging' of the probe surface using a surface composed of a series of sharp spikes. (V. Craig and D. Williams; C. Neto [University of Florence, Italy])

Anthony Hyde with the latest version of the surface force apparatus



Triplet of interwoven chiral 3D eucluidean networks derived from 2D hyperbolic surface tilings

Surface Force Measurements

The effectiveness of the recently developed Capacitance Dilatometer for the Surface Force Apparatus has been greatly enhanced by the implementation of new instrumentation and anti-vibration measures. Measurements have been made of the dispersion force between mica surfaces in air in the retarded regime with unprecedented accuracy and it is found that above 10 mm separation, Casimir-Polder theory that takes account of retardation fits the results much better than non-retarded van der Waals theory. (A. Stewart and V. Yaminsky)

Interfacial Friction

The interfacial friction between single crystal mica surfaces has been studied with the friction attachment for the Surface Force Apparatus, constructed in the Department. In contrast to ordinary friction which involves shear and fracture of asperities in the contacting surfaces, interfacial friction occurs without observable damage between the atomically smooth surfaces. A previously unreported peak has been detected in the interfacial friction of mica after the surfaces have been separated for only a few seconds and then brought together again and this has been correlated with the humidity of the experimental atmosphere. (S. Ohnishi and A. Stewart)

Theory of Atomic Forces and Intermolecular Interactions

It has been shown that in semi-classical electrodynamics, which describes how electrically charged particles move according to the laws of quantum mechanics under the influence of a prescribed classical electromagnetic field, only a restricted class of gauge transformations is allowed. This lack of full gauge invariance is due to the requirement that the scalar potential in the Hamiltonian of wave mechanics represent a physical potential. (A. Stewart)

Atomic Forces in Perfect Crystals

A generalised form of the Foremann-Lomer theorem that describes the properties of phonons in perfect crystals has been derived and explicit, exact and general relations in terms of atomic force constants have been found for deviations from the Blackman sum rule which itself is shown to be derived from the generalised Foreman-Lomer theorem. (A. Stewart)

Fundamental Molecular Interactions

Understanding of fundamental molecular interactions is important for many applications, e.g. catalysis. Resonance interaction between two atoms in an excited configuration is experimentally a "hot topic" with a crucial role in cold molecule formation. The textbook result for the resonance interaction used for interpretation is wrong. We have derived correct results for the retarded Casimir-Polder free energy between two ground-state molecules in a narrow cavity, and for the resonance interaction in free space and in a cavity. (M. Boström, J. Longdell and B. Ninham)

Specific Ion Effects: Why DLVO Theory fails for Biology

According to DLVO (Derjaguin, Landau, Verwey and Overbeek) theory, charge is the only relevant ionic property. However, biology is full of Hofmeister effects where different ion pairs (with the same charges) give very different results. The basic (DLVO) theory which underlies all of physical chemistry for the past 60 years turns out to be fundamentally wrong and thermodynamically inconsistent. A new theory has been developed that can accommodate many specific ion effects. Force measurements and ion binding are mutually inconsistent without taking the extra dispersion forces into account. (M. Boström, D. Williams and B. Ninham)

Latent Heat of Surface Fusion of Long-Chain n-Alkanes

The latent heat of surface fusion of long-chain n-alkanes is calculated from the temperature derivative of the measured surface tension between the bulk freezing and the surface freezing points. The calculated heat of fusion of crystalline n-octadecane monolayer is $\approx$150 J/g and that of n-eicosane is $\approx$140 J/g, close to the heat of fusion of bulk hydrocarbons and in excellent agreement with the recently reported calorimetry data. (N. Maeda and V. Yaminsky)

Experimental Observations of Surface Freezing

We have examined experiments on surface freezing within the wider framework of surface thermodynamics. Surface phase transitions, nucleation and crystallisation of bulk long-chain n-alkanes are discussed, with implications for capillary melting and freezing of substances at nanoscales. (N. Maeda and V. Yaminsky)

Hydrophobic Interactions

The long range hydrophobic attraction extensively studied over the past two decades can not be accounted for by modern theories of surface forces. We show here that bridging the surfaces by material of hydrophobic coatings and/or vapour cavities explains variable manifestations of the effect. The classical theory of capillary phase separation and vapour nucleation stays behind the experimental observations. Quantitative analysis of experimental force-distance profiles can be based on the equations that describe Laplace elasticity of bridging menisci of capillary condensates of vapours of wetting liquids and vapour cavities in non-wetting liquids. The attraction changes to repulsion when the confined bubbles, droplets and other protrusions from the surfaces are prevented from coalescence on approach. (V. Yaminsky and B. Ninham)

Hydrophobic Hydration

The problem of hydrophobic hydration is at the boundary line between solution chemistry and surface thermodynamics, with focus on water structure and applications to biological self-assembly. In this retrospective, we trace the origins of the idea and evolution of the term, analyse basic definitions, outline directions of research and consider current trends. The essential physics of hydrophobic phenomena follows on the lines of consideration for macroscopic and molecular cohesion and adhesion. (V. Yaminsky and B. Ninham)

Dynamic Wetting Transitions

Following the classical work of Thomas Young (1805), we provide exact experimental and theoretical solutions of the long-standing problem of contact angle hysteresis. The interfacial gauge condition of mechanical equilibrium and chemical coexistence at the three-phase line, the practical adsorption theory of static and dynamic dewetting, is thermodynamically based on the Gibbs adsorption equation. (V. Yaminsky; K. Eskilsson [Institute for Surface Chemistry, Stockholm, Sweden]; L. Ter-Minassian Saraga [JUPAC & CNRS, France])

The Interfacial Gauge

In the realm of thin films and colloids, the interfacial gauge condition accounts for the plethora of interfacial phenomena including Casimir-Lifshitz forces, DLVO and specific ion effects, molecular interactions in confinements, friction and hydrophobic transitions. The physics of chemically stagnant surfaces of solids has been placed on rigorous thermodynamic and molecular grounds. (V. Yaminsky, B. Ninham and S. Ohnishi)

Self-Adsorption

Through the definition of self-adsorption we extend the notion of Gibbs adsorption from solutions towards pure substances. The equation of state provides an experimental and theoretical account of the absolute value of surface energy of liquids and solids. The problems of surface entropy and condensed phase transitions, melting and crystallisation at surfaces and under confinement have been investigated. (V. Yaminsky and N. Maeda)

Satomi Ohnishi in the surface forces laboratory

Restricted Enzyme Activity

Specific ion effects are important parameters controlling the activity of restriction enzymes in biology. A hypothesis concerning the mechanism of restriction enzyme action emerges for the first time. (B. Ninham; H.K Kim and B. Nordén [Chalmers University, Sweden])

Bacterial Response to Surfactants and Biocides

Studies of protein expression of bacteria in response to surface attachment, biocide and cationic surfactants show that biocides and surfactants induce the same or similar responses. This was predicted. The ramifications for bacterial immunity are enormous and the work continues. (B. Ninham; P.O. Glantz and G. Svensäter [Malmö University, Sweden])

Novel Materials and Self Assembly

Echinoderm Skeletal Morphology

The complex fenestrated network of apparently crystalline magnesian calcite in the sea-urchin test (the hemispherical dome that supports the spines) is a spectacular example of biomineralisation: the growth of inorganic materials in vivo. We have prepared thin sections suitable for optical microscopy and transmission electron microscopy (TEM), thanks to the expertise of John FitzGerald. The relation between calcite crystal orientation and channel axes appears to be variable, and complex. TEM images at high magnification reveal the presence – in some regions only – of microscopic pores, likely pore networks, about 20 Å in diameter. We suspect those pores are the location of the elusive proteins known to be contained within the calcite. (J. FitzGerald [Research School of Earth Sciences]; G. Schroeder, A. Christy and S. Hyde)

The carbonate-silica trumpet bell viewed under polarised light

Growth and Form of Carbonate-Silica Biomorphs

In the past year, the work has focussed on the precipitation of barium carbonate at very low silica concentrations (down to hundreds of ppm silica). A new striking ultrastructural morphology, a trumpet bell, has been observed, in addition to the sheets and twisted ribbons we have been studying. A number of diffraction patterns have been collected (with mixed success) on the sheet and ribbon aggregates. The data confirms the formation of a novel material, with orientational ordering between the carbonate crystallites, but no translational order. Modelling of the expected diffraction continues. Data has also been collected on the growth rates of the ribbons as a function of temperature, and an activation energy of about 50 kJ per mole can be adduced. The resemblance to liquid crystals (particularly chiral examples such as the blue phase) is striking. (S. Hyde, A. Christy and N. Welham; J.M. Garcia Ruiz [Granada University, Spain])

Mesoscopic Modelling

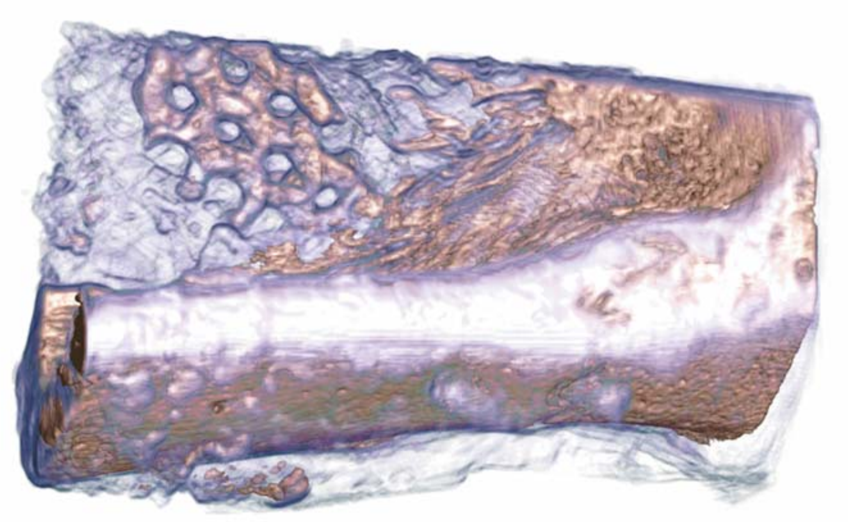
Using a classical density functional theory framework, we simulate the structure of quasi one-dimensional structures (e.g. micelles) on the mesoscopic level. The simulation tool allows the study of the effect of polydispersity on micelle structure, finding critical micelle concentrations, comparison to SAXS data, etc. Furthermore we are incorporating reaction kinetics into the model to be able to study the structure-dominated reaction mechanisms like, for example, emulsion polymerisation. (R. Sok)

Collapse of Copolymers

One of the key questions in biophysics and polymer physics is how primary chain structure (chain sequence) affects the collapse from a coil to a globular state. Our work attempts to answer part of this question by examining one of the most basic properties of a chain sequence, its degree of association between like monomers or "blockiness". Specifically, we use Langevin Dynamics to simulate the collapse of a model polymer with two monomer types, one of which is in a poor solvent and the other in a good solvent. The tendency for phase separation that is inherent in this system gives rise to some interesting phenomena such as the formation of intra-molecular "micelles" in the collapsed state. We also observe at least two distinct stages in the kinetics of collapse, which are related to phase separation at different length scales. The relative importance of these two stages depends on "blockiness" in the primary chain structure. (D. Williams and I. Cooke)

Paramagnetic Carbon Nanofoam

A new form of carbon material, a low-density cluster-assembled carbon nanofoam was produced in the ANU several years ago by high-repetition-rate laser ablation of a glassy carbon target in an ambient non-reactive Ar atmosphere. We discovered recently that along with many unique properties of the nanofoam (fractal structure, indications on the presence of hyperbolic surfaces, air-like density, diamond-like resistivity, high ratio of sp_3 to sp_2 bonds, and high density of unpaired spins) this pure carbon material possesses a strong paramagnetic susceptibility of about 0.01 of that for transition metals. The density of spins measured by ESR is 8.8×10^{20} spins/gram, suggesting strong paramagnetic



3D image of tissue engineered bone implant obtained by micro X-ray CT; the mineralised bone exhibits the polymer scaffold morphology within the implant region.

properties in striking contrast to diamagnetic properties of all known allotropes of carbon. The origin of this paramagnetic susceptibility can be traced to the complex microstructure of the nanofoam. (A. Rode [LPC], E. Gamaly, S. Hyde and A. Christy; R. Elliman [EME]; A.I. Veinger [Ioffee Physical-Technical Institute, Russia]; D. Golberg, [National Institute for Material Science, Japan])

Young's Modulus for Single-Walled Carbon Nanotubes: Scaling and Limits

An analytical scaling for Young's modulus of single-wall carbon nanotubes (SWNT) is developed on the basis of the empirical, atomic pair potential for graphite, and on linear elasticity. Young's modulus for a SWNT is explicitly expressed through Young's modulus for a defectless graphite mono-layer, the carbon-carbon binding energy, the tube wall thickness, and its radius, thereby revealing the physical reasons for the high stiffness of a SWNT. (E. Gamaly)

Cluster Ion Stopping and Fragmentation in Solids

A self-consistent model for the stopping of large energetic molecular cluster ions in solids is described. It is shown, in contrast to previous models, that the large cluster stopping occurs in a plasma created by the leading ions. Calculated stopping power, track widths and track lengths agree semi-quantitatively with experiments on the stopping of 40 MeV C_{60} molecular cluster ions in polycrystalline YIG (yttrium iron garnet). The essential 'carrot' shape of cluster tracks observed by TEM is due to progressive electron capture during slowing-down. We also show that the triggered avalanche of nuclear scatterings at a certain cluster velocity leads to a cluster splitting and the branching of tracks with a qualitative fit to the experimental data. (E. Gamaly; L. Chadderton [AMPL]; S. Cruz Jimenez [Universidad Autonoma Metropolitana, Iztapalapa, Mexico])

Structure and Phase Equilibria of Beryllian Sapphirine-Khmaralite

X-ray diffraction and transmission electron microscopy of synthetic Be-bearing sapphirine demonstrated the presence of the 2M polytype – a first for the synthetic mineral. Phase assemblages in synthetic products and comparison with natural rocks allowed modelling of the maximum Be content as a function of pressure and bulk composition. Extreme extension of the (sapphirine + forsterite) stability field due to the presence of Be, and located the absolute maximum of $(BeSi)(AlAl)_{-1}$ solid solution was found, lying at the MgO-BeO-Al_2O_3-SiO_2 univariant reaction (sapphirine + orthopyroxene + chrysoberyl) = (surinamite + forsterite). This reaction has not been located experimentally, but lies between 0.5 – 1.3 GPa pressure at 800 – 1000^{o}C. (A. Christy; Y. Tabira [Research School of Chemistry]; E.S. Grew [University of Maine, USA]; A. Hölscher and W. Schreyer [University of Bochum, Germany])

Shungite and Associated Phases

Characterisation of shungite, a rock composed primarily of dense glassy carbon, has focussed this year on the phases present as micron-scale inclusions and veinlet fills. Field-effect SEM, analytical TEM and Raman spectroscopy have been used to identify a suite of unusual Cr-V-Fe-Ni oxides, sulphides and silicates. (A. Christy)

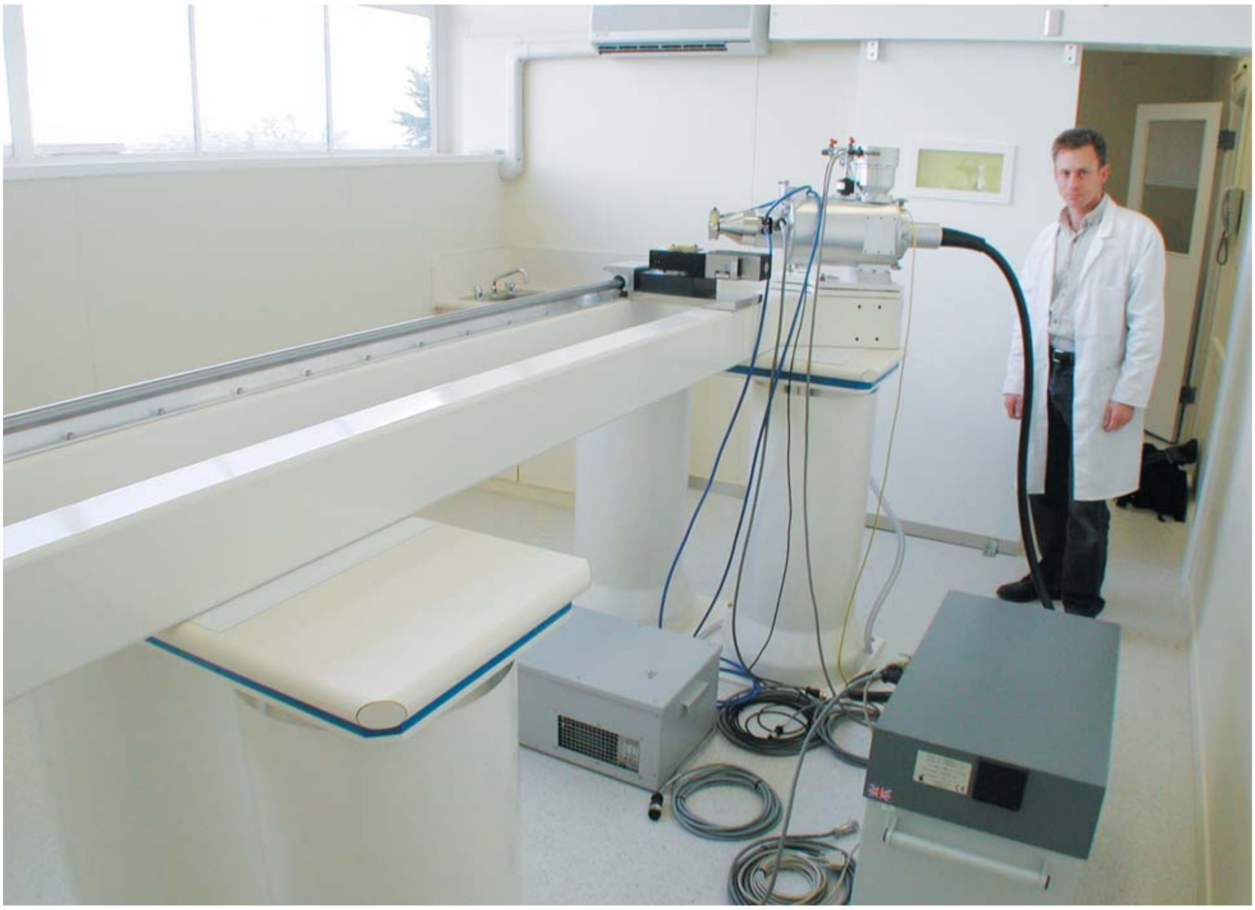
Synthesis of Novel Amorphous Nanoporous Silicates

Treatment of conventional silicate gels to make them partially hydrophobic before low-temperature hydrothermal treatment has been found to produce highly porous, homogeneous silicates that are completely amorphous to X-ray diffraction. The specific surface area of the product is similar to that of zeolites, but pores span a range of sizes from nanometres to hundreds of nanometres, and the framework incorporates a high proportion of octahedral as well as tetrahedral cations. (A. Christy, N. Welham and S. Hyde)

Random Materials

Characterisation of Disordered Materials

We have quantified random morphologies obtained experimentally from micro-CT (Computed Tomography) and for a range of disordered microstructural models utilising tools from integral, statistical and differential geometry and topology. We have developed a novel scheme which allows one to accurately reconstruct a Boolean composite media for all volume fractions from a single image. (C. Arns and M. Knackstedt; K. Mecke [Max Planck Institute for Metallforschung, Germany])



Tim Sawkins working on the assembly of the new high-resolution X-ray computed tomography facility

Interpretation of Laboratory Core Measurements

Worldwide, the petroleum industry spends in excess of a billion dollars annually on work related to the characterisation of reservoirs. A large part of this is spent on obtaining core material, performing tests and measurements on the core material and interpreting the test measurements in order to apply them to the field scale. A major uncertainty in the interpretations is the manner in which measurements on the core scale relate to the field scale. A significant reduction in this level of uncertainty is the goal of this project. Collaboration with BHP and access to their store of core material and accompanying database of laboratory measurements will provide an opportunity to probe the role of heterogeneity in determining petrophysical properties. (C. Arns, M. Knackstedt, A. Sheppard and R. Sok; W.V Pinczewski [UNSW]; G. Bunn [BHP Petroleum])

Development of the Virtual Materials Lab

Imaging materials via high-resolution X-ray CT and subsequent laboratory measurement of material properties will allow us to form a more accurate and comprehensive picture of the role of microstructure in governing the mechanical and transport properties of disordered materials. Simulations of the conductance, elastic and NMR properties of a suite of Fontainebleau sandstone samples obtained from the analysis of microtomographic images was compared to experimental results. The agreement is excellent. The ability to develop accurate cross-property correlations is underway. These results have elicited interest from companies worldwide. We have also begun a collaboration with BASF on characterisation and properties of foamed materials. (C. Arns, M. Knackstedt, A. Sheppard and R. Sok; W.V. Pinczewski [UNSW])

Fluid Penetration Mechanisms into Paper Products

Cryo scanning electron microscopy has been used to visualise the penetration of a wetting fluid into paper products. The observed fluid flow cannot be characterised by an advancing wetting front moving through the bulk of the pores. We observe a large and diffuse partially saturated zone, where fluid occupies only the edges of pores and forms films along channels formed by fibre overlaps. The results indicate that the fluid movement is primarily due to the advance of the wetting fluid in the form of bulk liquid films along these channels. This is in contrast to the common description of fluid penetration where the primary flow mechanism is based on the bulk filling of pores. An accurate description of paper web morphology and fluid penetration mechanisms gives a good mechanistic description of the fluid imbibition into unsized paper. (R. Roberts, T. Senden and M. Knackstedt; M.B. Lyne [International Paper])

Network Modelling of Capillary Dominated Fluid Displacements in Porous Structures: Role of Topology

The displacement of one immiscible fluid by another inside a porous structure occurs in many places throughout the earth's crust. Our understanding of what governs the displacement is still poor. We are using network modelling to better understand how the topology of the porous structure affects the displacement, and also to investigate the role played by long-range correlations of the material properties. (A. Sheppard, M. Knackstedt and R. Sok; J.-Y. Arns [UNSW])

Elastic Properties of Clean and Cemented Sandstones

Accurate elastic modulus-porosity relations are crucial in geophysical exploration studies. Unfortunately, experimental data are strongly scattered and offer poor correlations. We have studied the relationships for clean and clay-bearing sands and shown that many empirical models perform poorly. Based on the simulation results we derive an empirical relationship for elastic properties of sandstones made up of multiple mineral phases. Comparison to several experimental studies gives an excellent match. (C. Arns and M. Knackstedt; W.V. Pinczewski [UNSW])

Equivalent Networks for Porous Rocks

Network model equivalents of numerous samples of sandstone obtained from the analysis of microtomographic images have been generated. We find that the description of the network topology is particularly crucial in accurately predicting multiphase flow properties. We are attempting to generate stochastic networks with topological properties representative of real sedimentary rocks. Accurate characterisation of the network topology requires the introduction of longer bonds, thereby satisfying higher order topological measures than connectivity alone. Measurements of pore geometry and correlations that occur at the pore scale in sedimentary rocks have also been made. (V. Robins, A. Sheppard, R. Sok and M. Knackstedt; J.-Y. Arns [UNSW])

Development of a High-Resolution X-Ray Computed Tomography Facility

The construction of a high-resolution X-ray CT facility is almost complete. A leaden room with safety interlocks, control systems and equipment infrastructure is now installed and the facility is undergoing final testing and calibration. The micro-focus X-ray source, precision rotation stage and scintillator-coupled 2048x2048 pixel CCD array will work in unison to produce X-ray attenuation projection data. Single data sets up to 14 GByte each can be collected within a day. The attainable resolution is expected to be <5 μm^3, using cone-beam geometry and specialised reconstruction algorithms based on the work of Per-Erik Danielsson at Linköpings University. A suite of computer programs have been written to process and visualise the collected projection data and to generate a 3D density and morphology distribution map of the specimen being analysed. (T. Sawkins, A. Sakellariou and T. Senden; M. Blacksell [Electronics Workshop]; B. Danaher [Mechanical Workshop])

Computational Geometry and Topology

Characterisation of Disordered Structures: Point Patterns

We are investigating the links between integral geometric measures and topological measures, particularly the Betti numbers, for disordered structures. To date, we have looked at Poissonian point patterns. (V. Robins; K. Mecke [Max Planck Institute for Metallforschung, Germany]).

Euclidean 3D Networks

Our project to generate and catalog networks continues. The development of general software to handle 2D hyperbolic symmetry groups (orbifolds) and group-subgroup relations is now in place. A general visualisation package that simultaneously displays orbifold symmetries in the hyperbolic plane (allowing toggling between the Klein and Poincaré disc models), and admits mapping of motifs onto the plane with those symmetries, as well as projections onto either the P, D or Gyroid triply periodic minimal surfaces has been completed. (S. Hyde; S. Ramsden [Vizlab, ANU Supercomputer Facility])

Medial Surfaces and Skeletons

The reduction of complex 3D morphologies to manageable structural representations is critical to the goal of precise quantitative structural description. Hyperbolic surfaces, with complex networks of labyrinths, can be exactly reduced to their medial surfaces. These are defined as the loci of centres of balls within the labyrinth spaces that tangentially coincide with the original surface at more than one point. The medial surface, coupled with the ball radius at each point (the Euclidean Distance Map) is an exact surface descriptor. Software has been developed to compute the medial surface and EDM for an arbitrary starting

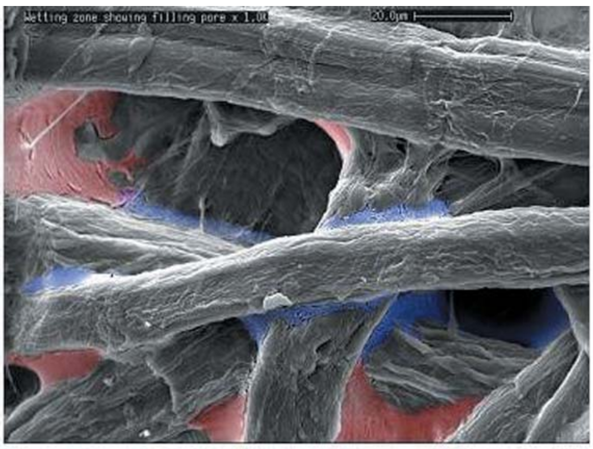


Illustration of the fluid distribution in paper fibre webs on wetting surface. In addition, we seek a useful and robust definition of the labyrinth skeleton. (G. Schroeder, A. Sheppard and S. Hyde; S. Ramsden [Vizlab, ANU Supercomputer Facility])

Protein Surface Structures

The tools developed to quantify curvature for arbitrary surfaces have been extended to "fit" surfaces through arbitrary point clouds. We have searched the Protein Data Base, and calculated the surface curvatures for many proteins, assuming a minimal neighbouring (but non-adjacent carbon numbers on the chain) α-carbon distance to define a surface. The results are being collated. Orientation of the surface patches, via the carbon number, allows separation of distinct structural motifs. The α-helix and parallel and anti-parallel β-sheet motifs are clearly identified from the histogram of surface curvatures. (Y. Nagai [Kokushikan University, Japan]; S. Hyde)

Software for the Skeletonisation of Very Large Tomographic Images

The Department's X-ray CT machine (under construction) will produce very large 3D images of porous and multiphase materials. We wish to analyse the topological and geometric properties of these materials. This analysis rests upon skeletonisation (also called medial axis extraction) in which a 3D contiguous volume region in the tomographic image is reduced to a 1D line network, known as the skeleton. We have developed several new algorithms for this purpose. (A. Sheppard, R. Sok and A. Sakellariou; B. Lindquist [State University of New York at Stony Brook, USA])

Analysis of Network Topology

Networks are ubiquitous in nature. In addition, many composite structures can be understood through the analysis of their skeleton, the network that reflects their connectivity. Despite this, very little attention has been paid to the characterisation of networks or how network characteristics affect the macroscopic properties of the structure. We are deriving measures for the characterisation of network topology and investigating how these measures correlate to macroscopic properties. (V. Robins, R. Sok and A. Sheppard)

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Atomic & Molecular Physics Laboratories

Dr Brenton Lewis
Head of 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.

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

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, positrons, and photons with atoms, molecules, and solids, in order both to further our understanding of the fundamental processes, and to provide information that is critical to an understanding of the applications.

There has been considerable staff turnover and rearrangement in the Department this year. Following the elevation of Professor Stephen Buckman to the position of Associate Director (Academic), Dr Brenton Lewis was appointed as Head of Department in October. In addition, Dr Maarten Vos' QEII Fellowship was converted into a standard appointment, as was the position of Dr Anatoli Kheifets (jointly with the Department of Theoretical Physics) who was also promoted to Senior Fellow. Drs Truscott, Sashin, Cavanagh, and Kono were appointed to fixed-term positions, the latter two funded by the ARC and the IPC, respectively, more than counterbalancing the loss of Drs Gulley and Hoogerland. In addition, Dr Robert Robson was appointed as a new Visiting Fellow (jointly with the Department of Theoretical Physics) and, in the technical area, Gary Picker was seconded from the Mechanical Workshop to replace Kevin Lonsdale.

A summary of the various research activities in the Department follows below. Highlights include: the development of a new method for detecting the vibrational motion of light elements, based on large-angle elastic electron-nucleus scattering; the first measurements of electron scattering from trapped metastable helium atoms; the design and construction of a new Toroidal Electron Spectrometer which achieves three orders of magnitude improvement in sensitivity over conventional devices; the first demonstration of completely destructive quantum interference between resonances in molecular predissociation. In addition, Professor Buckman participated in exciting, ground-breaking research on positron scattering during his year-long tenure at UCSD on a Fulbright Senior Fellowship.

Finally, members of the Department were again successful in winning grants, awards and other marks of distinction during the year. Professor Erich Weigold and Dr Julian Lower were awarded a RIEF Grant (jointly with Flinders University) and an Australian-German Collaborative Grant; Professor Buckman won a RIEF Grant (jointly with the University of Western Australia); and Dr Lewis (with Drs Baldwin and Gibson) won an ANU Major Equipment Grant for the purchase of an excimer laser. Professor Weigold and Dr Robson took up Humbolt Fellowships during the year. Dr Lewis was elected to Fellowship of the American Physical Society and successfully presented a bid to host the VUV14 International Conference in Australia in 2004.

Experimental

Atom Manipulation

The atom manipulation project is a joint program between AMPL and the Laser Physics Centre which uses laser cooling and trapping techniques, both to study fundamental atomic- collision physics, and also to investigate applications of atom-optical elements to new devices on nanometre scales (see LPC annual report).

In the collision studies, the major development this year has involved the first experiments on electron scattering from trapped metastable helium atoms. We employed our bright atomic beam line to load a magneto-optic trap with ~ 10^8 helium atoms in the 2^3S_1 excited state, and cooled the atoms to around 1 mK. A further optical-molasses stage cooled the atoms to several hundred mK.

This additional cooling step is crucial to extend the lifetime of the atomic cloud which we detect using a further probe laser beam. We employ RF spectroscopy, detuned from the 1083 nm 2^3S_1 - 2^3P_2 trapping transition to provide a non-destructive measurement of the number of helium atoms within the probe laser-beam volume. Measurements can thus be made of the number of trapped atoms over tens of milliseconds, prior to ballistic expansion of the atomic cloud outside the probe beam.

The atomic cloud (initially 8 mm in diameter) is intersected by a 20 mm-diameter electron- beam current of around 100 mA. We measure the total trap loss due to electron collisions and thereby determine the total electron scattering cross section as a function of electron energy. The use of laser-cooling and -trapping techniques has allowed us to obtain, for the first time, absolute cross-section measurements in the 10 – 100 eV energy range for He in the 2^3S_1 metastable state. As shown in the accompanying figure, these measurements allow a direct comparison of the total scattering cross sections with the latest theoretical predictions. (M. Colla, R.G. Dall, L.J. Uhlmann and S.J. Buckman; K.G.H. Baldwin [LPC])

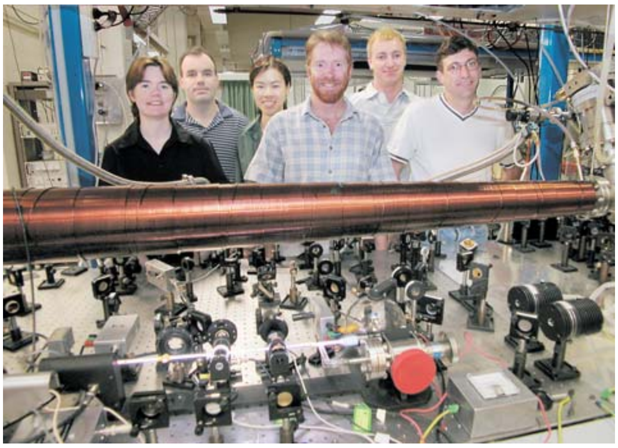
Positron Scattering

As part of a collaboration with colleagues at the University of California, San Diego, during an extended outside-studies program, a series of ground-breaking experimental measurements have been made of low-energy positron scattering from atoms and molecules. Using a high resolution (~ 25 meV) positron beam from a Penning-Malmberg trap, the first measurements of state-specific, absolute cross sections for the electronic excitation of Ar, H_2 and N_2 have been made. This technique was also used to investigate low-energy elastic scattering and vibrational excitation in a range of atoms and molecules. (S.J. Buckman; J.P. Sullivan and S.J. Gilbert; C.M. Surko [University of California, San Diego, USA])

Electron Momentum Spectroscopy (EMS) of Solids

A lot of attention has been paid to fine-tuning the spectrometer. The energy resolution has been improved from 2 eV to 1 eV in coincidence mode. In singles measurements, the 25 keV electrons can now be analysed with an energy resolution of 0.4 eV.

Improving the energy resolution has led to some new physical insights. It has become obvious that elastic-scattering spectra contain additional information about the sample composition (especially the light elements such as H) and the (vibrational) kinetic energy of the target atoms. Previously, this type of



Members of the Atom Manipulation Group with the beam line

information could only be obtained using energetic neutrons, in experiments that require a huge infrastructure.

The resulting spectral momentum densities, as measured by EMS, show an increased contrast, making comparison with theory (A.S. Kheifets) more straightforward. A polarised electron source has been designed and will be constructed in the coming year. It is expected to improve the energy resolution as well as the study of spin asymmetries in the energy-resolved momentum densities. (V. Sashin, M. Vos and E. Weigold)

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

The process of electron-impact ionisation is of importance, both from a technological and a fundamental perspective. In the former case, electron-impact ionisation plays a pivotal role in determining the behaviour of such systems as lasers, plasmas and gas discharges. Thus, an improved understanding of this process contributes to the development of devices based around these systems. In the latter case, electron-atom collisions provide an ideal test bed to probe the many-body behaviour of a system of interacting electrons which forms the basis of the electronic structure of matter.

Our experiments employ nanosecond timing techniques to detect pairs of electrons emerging from single-collision events in which the magnetic-projection states of the reaction participants are prepared by laser techniques prior to the collision. Whilst our experiments to date have been very successful in revealing new effects in electron-atom collisions, low count rates have limited the measurement precision. For this reason, we have completely rebuilt the apparatus over the last few years, employing new

Panorama of the atom manipulation laboratory technology based on toroidal analysers, differential pumping of the atomic target beam, and state-of-the-art picosecond timing detectors. This construction phase is now complete, with improvements in efficiency of between three and four orders of magnitude over our former technology anticipated within the next few months. (J.C.A. Lower and E. Weigold)

Microscope for Atomic Collisions

Experiments in which atomic and molecular structure and collision dynamics are explored normally involve the overlap of projectile and target beams, with spectrometers used to energy- and momentum-analyse the reaction products. Conventional spectrometers measure only a small fraction of the total scattered particle flux and must sequentially scan through the energy and momentum coordinates to obtain some overview of all of the possible reaction outcomes. In addition to the inefficiencies associated with sequential data collection, many momentum coordinates remain inaccessible due to mechanical constraints, and separate detectors are required for the measurement of multiple reaction products.

In the present program, supported by the ANU Major Equipment fund, we intend to develop a new-generation spectrometer in which all reaction products are measured on a single detector and data are collected over all energy and momentum coordinates, simultaneously. The spectrometer is to be based on the time-of-flight (TOF) technique, in which the momenta and energies of particles are determined by their drift times from the collision volume to the detector. The first phase of this project was initiated this year through the development of a fast, pulsed-beam source of electrons. The next phase will involve the installation of our new TOF spectrometer for the simultaneous measurement of energy and momentum information.

This technology, once developed, will enable experiments of greatly enhanced kinematic range, speed and precision, and will open the door to experiments on reactive targets which presently remain unfeasible. (J. Harrison, R. Panajotovic, J.C.A. Lower and S.J. Buckman)

VUV Molecular Spectroscopy

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

The (0,0) band of the magnetic-dipole transition $^3\Pi_g$- $X^3\Sigma_g^-$ of the oxygen molecule has been discovered and characterised through a series of measurements using the 2.2 m monochromator system. Based on these measurements, the contribution of this transition to the unassigned continuum underlying the atmospherically-important Schumann-Runge bands has been estimated. (E.H. Roberts, B.R. Lewis and S.T. Gibson; K. Nixon [Flinders University])

This year we have completed the experimental program of high-resolution vacuum-ultraviolet (VUV) laser absorption studies of diatomic oxygen in the Schumann-Runge band system near the dissociation limit at 175 nm. These studies have employed VUV radiation generated using difference-frequency four-wave mixing techniques in Xe (the nonlinear medium) to yield Doppler limited (< 0.1 cm^{-1}) bandwidths. Work has also commenced on using liquid-nitrogen-cooled gas samples to provide temperature-dependent data. As the tunable VUV radiation excites increasingly higher vibrational levels, the complexity of the spectral lines near the continuum is enriched by perturbations between coincident energy levels from different electronic states. The perturbing effect on the line positions, strengths and widths has already led to the identification of a new electronic state of O. We have also shown that the rotational dependence of the triplet-splitting constants λ and γ for B(v=22) exhibit a sign reversal due to the change in the sense of the perturbation by the $C'\ ^3\Pi_u$ state. This result is in good agreement with our theoretical modelling. Further assignment and modelling of the experimental spectrum will yield a definitive database for this important atmospheric band system. The VUV laser-spectroscopic measurements reported here have recently been supported by the appointment of a new PDF position in the IPC-funded Solar-Terrestrial Environmental Program. (K. Waring, M. Kono, B.R. Lewis and S.T. Gibson; K.G.H. Baldwin [LPC])

Resonance-Enhanced Multiphoton Ionisation (REMPI)

Analysis has been completed of (2+1)-photon REMPI spectra from the $X^3\Sigma_g^-$ state of O_2 which reveal transitions into the $3p\pi_u\ ^3\Delta_u$ Rydberg state for the first time, such transitions being forbidden in one photon spectroscopy. The observed predissociation has been used to produce a model of the Rydberg-valence interactions for the $^3\Delta_u$ states. (B.R. Lewis, S.T. Gibson; R.A. Copeland [SRI International, USA])

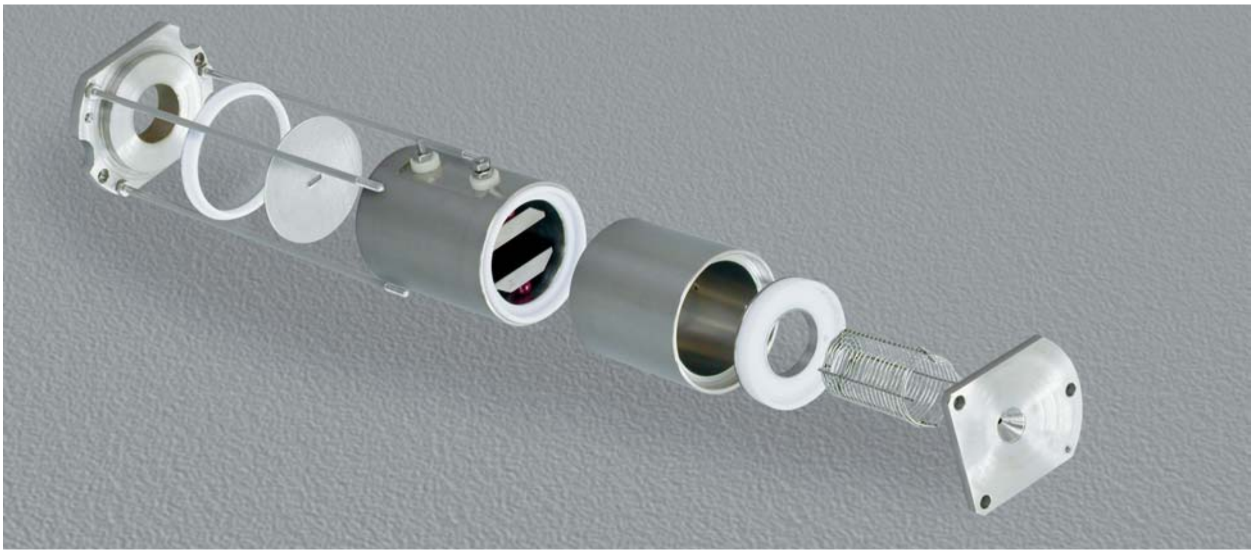
New, properly calibrated (2+1)-photon REMPI spectra from the metastable $a^1\Delta_g$ and $b^1\Sigma_g^+$ states of O_2 have been acquired and analysed rotationally, yielding the first accurate experimental information on strong perturbations in the Rydberg $d\ ^1\Pi_g$ state. This information will be used to optimise a new coupled-channel treatment of the $^1\Pi_g$ Rydberg-valence interactions in O_2. (B.R. Lewis and S.T. Gibson; R.A. Copeland [SRI International, USA]; M.L. Ginter [University of Maryland, USA]; J.S. Morrill [Naval Research Laboratory, USA])

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

Molecular Photodissociation Dynamics

This year has seen significant technological advances in the design and construction of the Coincidence Photofragment/Photodetachment Spectrometer. Details of a novel bunching, gating and re-referencing unit, developed to control the ion-beam packets, have been published.

The final component necessary to perform photodetachment/photoelectron spectroscopic experiments is a detector to energy analyse the photoelectrons. Computational simulations have indicated that, with careful design, the technique of velocity image mapping will provide considerable advantages over conventional TOF techniques. This scheme is being implemented in the current design. A low-cost phosphor detector has been constructed to image the velocity distributions. The phosphor preparation incorporates the use of a thin epoxy layer, using dope



An expended view of the fast electron pulsing unit

commonly used in the construction of ultralight model aeroplanes. This detector will have a dual role, since it will also be used to record the production of photofragments. The first experimental measurments using the spectrometer are expected next year, following the replacement of an excimer laser through a successful ANU Major Equipment bid this year. (S.T. Gibson, B.R. Lewis, S.J. Cavanagh and E.H. Roberts; K.G.H. Baldwin [LPC]; C.M. Puetter [Physics, Faculties]; R.G. Elliman [EME])

Atoms, Molecules, Radiation and the Nanoworld

In studies of the interaction of radiation with matter, we have continued to clarify those processes in which energy deposited in a solid is converted into defects, the mechanisms for latent track registration (the physics of particle detectors), and the atomic and molecular physics of condensed-matter phase changes. Specifically, we find (using TEM) that GeV heavy ions produce intermittent tracks in LiF composed of intermittent cubic lithium nano-colloids (c.f. CaF_2). This, and earlier observations, made necessary an entirely new microscopic model for damage creation, and heavy particle track registration, in solids generally. This model is based on defect diffusion physics quite specific to each target and Bravais lattice. It finally replaces old macroscopic 'thermal spike' concepts which are most frequently invalid. (L.T. Chadderton; C. Trautmann [GSI, Germany])

Two new fission-fragment track programs are underway. The first concerns natural radioactivity in precious opal, and therefore opal exploration, and also growth of photonic band-gap artificial opal for IT applications. The second is a long study of the natural mineral apatite, its response to fission fragments, to anomalous track-length shrinkage under varying temperature and pressure conditions, and its use in geothermometry. (B. Senior, Senior and Associates, Canberra; R. Jonckeere [MPI, Germany]; A. Wendt [University of Cambridge, UK]; L.T. Chadderton)

Further studies of molecular self assembly by heterogeneous nucleation have shown that foreign nuclei behave in a fluid manner during catalytic capillary growth of C and BN nanotubes. Skeletal nanotubes can be formed with metallic nuclei repeated at each knot. We investigate the electronic and mechanical properties of these new species in nanotechnology. (J. Williams and C.Ying [EME]; L.T. Chadderton)

Theoretical/Computational

Electron Interactions with Atoms

The relativistic distorted-wave method was used to calculate the Stokes parameters associated with the excitation of the D states of Mg. These calculations were performed in advance of an anticipated experiment. Similar calculations for the Group IV elements, C, Si and Ge, and Zn have also been completed.

Theoretical work has commenced on the numerical calculation of relativistic Coulomb functions to be used in a new relativistic distorted-wave program for the excitation of heavy ions. (R.P. McEachran; A.D. Stauffer [York University, Canada]; R. Srivastava [Roorkee University, India])

The treatment of electron exchange in low-energy electron-impact ionisation of the inner and outer shells of Ar has been initiated. Although considerable progress and understanding of this process has been made, the overall agreement with experiment is not yet satisfactory. (R.P. McEachran; D.H. Madison and D.A. Biava [University of Missouri-Rolla, USA]; B. Lohmann and M.A. Haynes [Griffith University])

The Sherman function for the elastic scattering of electrons from Kr has been determined and the results compared with the current experiment being conducted at Griffith University. So far, the agreement between experiment and theory is far from satisfactory. Further investigations on both fronts are presently underway. (R.P. McEachran; B. Lohmann, W.R. MacGillvray and M.R. Went [Griffith University])

Multiple Atomic Ionisation

Multiple atomic ionisation following the absorption of a single photon or a knock out by a fast projectile is a dynamic, vibrant and controversial field of atomic-collision physics. Because of the pivotal role of electron-electron correlations, these processes continue to receive considerable attention, both theoretically and experimentally.

The close-coupling theory of multiple atomic ionisation has been further extended. The roles of various correlation mechanisms have been uncovered in the double photoionisation of the He atom. The cross-over between the shake-off and two-step mechanisms has been predicted theoretically and confirmed experimentally. Full parametrisation of the symmetrised double-photoionisation amplitudes has been achieved, offering a general description of the double photoionisation process over a very wide range of photon energies and geometries of the two-electron escape. Second-order corrections to the electron-impact ionisation process have been estimated in the case of double ionisation of the He atom. (A.S. Kheifets; I. Bray [Murdoch University])

Positron Interactions with Atoms

The excitation cross sections to the 6s, 7s, 5d, 6d and 7d levels of Xe have been determined within a distorted-wave framework in an energy range up to 200 eV. When combined with previous work on the elastic and ionisation cross sections, as well as the Ps formation cross section, these results are in satisfactory agreement with experimental measurements of the total cross section. (R.P. McEachran; L.A. Parcell [Macquarie University]; A.D. Stauffer [York University, Canada])

A new model for the determination of positron ionisation cross sections has been developed and tested on H and the noble gases. With the exception of Ne, this new procedure gave very good overall agreement with experiment. (R.P. McEachran; R.I. Campeanu [Seneca College, Canada]; A.D. Stauffer [York University, Canada])

The relativistic distorted-wave method was used to determine the excitation cross sections to the two 4s (J=1) fine-structure levels of Ar. These results are in quite good agreement with the first positron experiment to measure cross sections to individual fine-structure levels of any atom. (R.P. McEachran; A.D. Stauffer [York University, Canada])

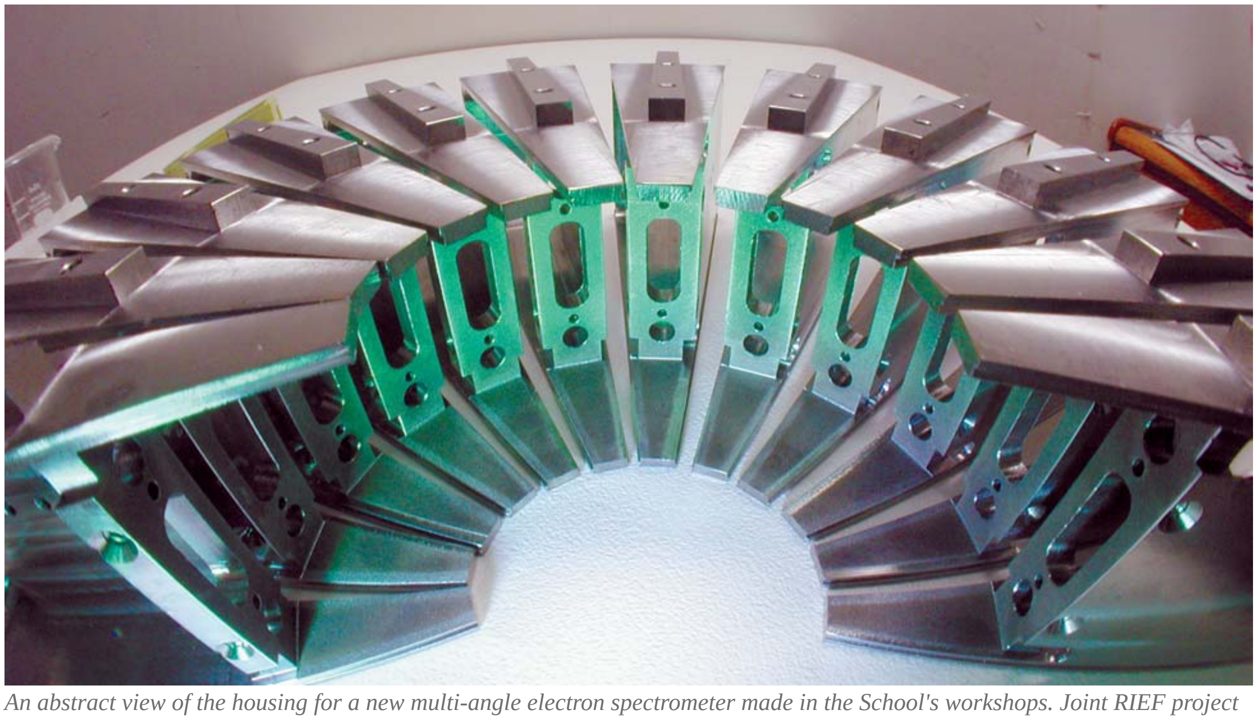
Many-Electron Correlations in Solids

Realistic models of many-electron correlations in 3D solids can now be implemented using efficient algorithms on high-performance computers. An accurate evaluation of the self-energy operator with screening of the interelectron interaction and vertex corrections can now be done on the basis of linear muffin-tin orbitals. This computational scheme has proven to be very successful in describing the spectral functions of various crystals composed of light s and p-electron atoms. Now this method is extended to heavier d-electron systems (Cu and Au). The calculated spectral functions have been favourably compared with experimental results from the EMS group in AMPL. (A.S. Kheifets; F. Aryasetiawan [JRCAT, Japan])

Close-Coupled Molecular Spectroscopy

Our close-coupling code for the treatment of interactions between molecular electronic states continues to provide invaluable research insight, contributing to eight articles published or accepted this year. Subjects treated include: line-shape asymmetries and photodissociation cross sections in the Schumann-Runge bands of O_2; intensity anomalies in the EELS of interacting Rydberg and valence states; completely destructive quantum interference between rotational predissociating resonances; Rydberg-valence-induced predissociation in the $3p\pi_u$ $^3\Delta_u$ state of O_2; anomalous isotopic predissociation in the $F\ ^3\Pi_u$ (v=1) Rydberg state of O_2; and Rydberg-valence perturbations in the $^1\Pi_g$ states of O_2. (B.R. Lewis and S.T. Gibson)

Dissociation of N_2 is an important process initiating chemical reactions in the upper layers of the terrestrial atmosphere. Excited singlet states accessible through dipole-allowed transitions from the ground state can energetically predissociate to the lower dissociation limits only through interactions with triplets which are comparatively poorly characterised at present. We have started a collaborative computational program to study the $^3\Pi_u$ states of N_2 using ab initio and close-coupling techniques in order both to characterise their mutual interactions and also to compute the predissociative effects of their spin-orbit and rotational interactions with the singlet states. (B.R. Lewis and S.T. Gibson; J.-M. Robbe [Univerisité de Lille, France]; H. Lefebvre-Brion [Univeristé de Paris-Sud, France])



An abstract view of the housing for a new multi-angle electron spectrometer made in the School's workshops. Joint RIEF project with Flinders University

Atmospheric Computation

Work has continued on an ARC-funded project involving quantum-mechanical modelling of the transmission of solar VUV radiation through the terrestrial atmosphere. Considerable progress has been made towards the ultimate aim of the project, i.e., to produce a comprehensive database to be used extensively by the community of atmospheric geophysicists in their photochemical models. The atmospheric transmission calculations are being tested against new, high-resolution cross sections performed in our VUV laser-spectroscopy laboratories. (B.R. Lewis and S.T. Gibson; L.W. Torop [Adelaide University])

Atmospheric Evolution, Tectonic Cycles and Climate Change

Conventional stellar theories suggest that the Sun has brightened by about 30% since it first joined the main sequence some 4.6 Gyr ago, but Precambrian glaciations are rare and there is no geological evidence for a totally frozen Precambrian Earth. One way of resolving the "faint young Sun" paradox is to assume that compensation for the faint young Sun is provided by a rich CO_2 – H_2O palaeo-greenhouse. On this basis, we have explored broad features of the long-term evolution of the Earth's climate using a 1-D radiative convective model, with negative feedback provided by temperature-dependent CO_2 weathering. The model balances contributions to the surface temperature from a steadily brightening solar flux against those from a generally diminishing CO_2 – H_2O palaeo-greenhouse. The steady brightening of the solar flux is the major external factor forcing atmospheric evolution and consequential climate change. Climate change also occurs in response to internal factors, including variations in the gas emission rate and physical and biological changes in the planetary surface.

As the Earth evolved with time, the model calculations suggest that the system passed through three qualitatively different "Megaclimates".

Megaclimate 1, with its high but declining surface temperatures, resulted from rapid outgassing in the early Archean combined with small weathering rates on a largely water-covered planet.

Megaclimate 2 commenced about 3 Gyr ago when weathering rates increased as major continental land masses began to be formed. The rarity of Precambrian glaciations and their restriction to two periods, one in the early (2.3 Gyr BP) and the other in the late Proterozoic (900 Myr ago), is explained by the increase in surface weathering rates that began about 1 Gyr ago with the transition from the Proterozoic to the Phanerozoic. Glaciations did not occur between 2 Gyr and 1 Gyr BP because the Sun brightened sufficiently in that interval to compensate for the CO_2 depletion caused by the growth in the continental land mass. Glaciations only recurred when weathering rates increased by further biological evolution. Plate tectonics, driven by convective cycling in the mantle, is included in the model through the Phanerozoic Supercycle (PSC) which describes idealised features of the assembly, stasis, fragmentation, dispersal and reassembly of supercontinents. The PSC has a period of about 300 Myr. We have found that modulation of the gas emission rate with a period of 150 Myr (one half that of the PSC) can account for the remarkable regularity of the sequence of major glaciations between 900 and 300 Myr BP. The model can be used to explain the late Cenozoic glaciation at about 35 Myr BP.

Megaclimate 3. Extending the model to the future suggests that the present CO_2 level is too low to compensate for the continued brightening of the Sun, leading to the steadily increasing surface temperatures of Megaclimate 3. (J.H. Carver; I.M. Vardavas [University of Crete, Greece])

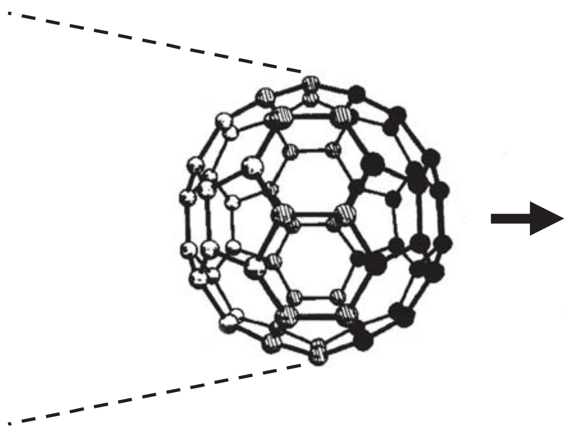
Atoms, Molecules, Radiation and the Nanoworld

Rules of additivity for the electronic stopping power of swift, heavy particles in mixed atomic gases do not apply, because atoms in solids and, therefore, collisions can be too close to each other (real bonding), yielding correlations (a first step from chaos into order) and because simultaneously there are excitation processes which end, not with free electrons, but with specific lattice-defined atomic motion. We have described this analytically for the first time. An additional 'interference' integral in the stopping-power expression can be dominant.

A proposed so-called new 'velocity effect' in electronic stopping powers (same stopping at two discrete velocities) has advanced in the literature without criticism. We have shown that this is the normal well-known velocity effect (across the Bethe-Bloch curve) expressed only at the target entry surface, where electronic sputtering (momentum dependent) takes place in a "Coulomb explosion". (L.T. Chadderton)

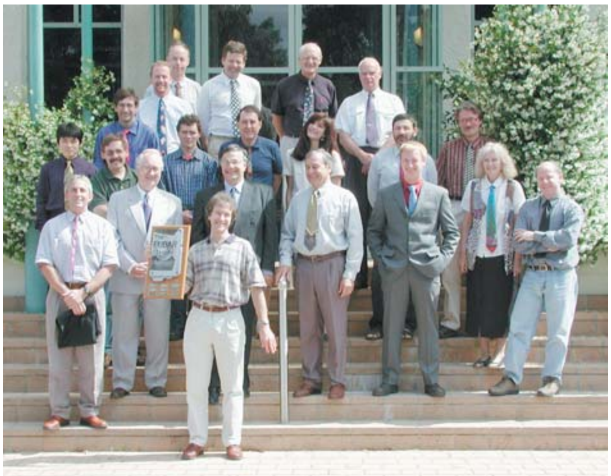
40 MeV C_{60} and other cluster ions produce carrot-shaped tracks in, e.g., YIG (yttrium iron garnet). We have explained the track characteristics; width, length, break-up, etc., in terms partly of plasma induction by the leading part of the projectile itself (see Figure), which hugely increases the total projectile effective charge.

This is a new, second electronic vicinage (neighbourhood) effect with a steric origin. Also uncovered is an entirely new steric nuclear vicinage effect, which leads ultimately to break-up of the projectile due to onset of an internal atomic displacement avalanche in the projectile itself, and to sub-track formation (c.f. fission). (L.T. Chadderton; E. Gamaly [AM]; S.A. Cruz [Ixtapalapa, Mexico])



Molecular C_{60} ion meteor creates hot plasma in a solid through which it then must pass. This is a new 'electronic vicinage effect'. (Gamaly, Cruz and Chadderton)

Double rainbows in the scattering of low-energy electrons are inverse vicinage phenomena in physics. A well-defined atomic bond length is, therefore, also a first step from chaos into order. Introduction of further order; triatomic, planar (e.g., benzene) and spherical (e.g., fullerene) molecules, and finally crystals (a well-defined lattice spacing) is accompanied by new rainbow-like phenomena in reciprocal space. We find it possible in this way to erect the Bragg law of diffraction by summing over rainbow-like scattering from individual atoms. (L.T. Chadderton and S.J. Buckman; S.A. Cruz [Ixtapalapa, Mexico])



Presentation of the annual "fubar" award to Julian Lower for sustained and excellent laboratory performance

Diffusion of Meteor Trails

The study of the diffusion of electrons in meteor trails has continued through this period. Calculations based on the theory of the ambipolar diffusion of meteor trails in the presence of the Earth's magnetic field have been made as a function of height above the Earth. This study, which is a significant advance on previous such descriptions, is based on an approximate swarm theory known as momentum-transfer theory. To carry out calculations on the trails it is necessary to have available values of the collision frequency (as defined in this approximate theory). These values have been computed using the best available momentum-transfer cross sections for O_2 and N_2. A paper on this work was presented at the Meteoroids 2001 conference, held in Finland in August. (M.T. Elford and R.E. Robson; K. Kumar [TP]; W.G. Elford [Adelaide University])

Staff

Senior Fellow and Head of Laboratories
Brenton Lewis, PhD DSc Adel, C Phys, FInstP, FAPS, FAIP (from October; acting Head until October)

Professors
Stephen Buckman, BSc PhD Flind, FAPS, FAIP (Head of Laboratories until October)
Erich Weigold, BSc Adel, PhD, FAA, FTSE, FAPS, FAIP

Adjunct Professors
Lewis Chadderton, DSc Dur, MA PhD Camb, C Phys, FInstP, FAIP
Robert McEachran, MSc PhD UWO, C Phys, FInstP

Senior Fellow
Anatoli Kheifets, BSc PhD St Pet (jointly with Theoretical Physics) (from July)

Fellows
Stephen Gibson, BSc PhD Adel
Anatoli Kheifets, BSc PhD St Pet (jointly with Theoretical Physics) (until July)
Maarten Vos, MSc PhD Gron (from July) (QEII Fellowship until July)

Research Fellows
Mitsuhiko Kono, MS Kyoto IT, PhD Grad U Adv Sci (from May)
Julian Lower, BSc PhD Flind
Andrew Truscott, BSc PhD Qld (from November)

Postdoctoral Fellows
Steven Cavanagh, BSc PhD Griff (ARC Fellowship) (from May)
Robert Gulley, BSc Qld, PhD (ARC Fellowship) (until February)
Radmila Panajotovic, MSc PhD Belgr
Vladimir Sashin, BSc Mosc (from September)

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Robert Crompton, BSc PhD Adel, AM, FAA, FInstP, FAPS, FAIP (Emeritus Professor)
Malcolm Elford, BSc PhD Adel
Mitsuhiko Kono, MS Kyoto IT, PhD Grad U Adv Sci (until May)
Hélène Lefebvre-Brion, DSc Paris (February-March)
Roland Lefebvre-Brion, DSc Paris (February-March)
Robert Robson, BSc Qld, DipMetB MetTs Melb, PhD, FRMS, FAPS, FAIP (jointly with Theoretical Physics) (from March)
Helge Skullerud, DTech Trond (September-November)
Glenn Stark, BS MIT, MA PhD UCB (August)

Senior Technical Officers
Stephen Battisson, AssocDipMechEng CIT
Graeme Cornish, AssocDipMechEng CIT
Colin Dedman, AssocDipSciInst Bdgo CAE
Kevin Roberts, MechTechCert SAIT

Technical Officer
Gary Picker, AssocDipMechEng CIT (from April; seconded from MWS)

Departmental Administrator
Alice Duncanson

Director's Unit

Professor Yuri Kivshar (top) and Professor John Love - Joint heads of Director's Unit

The Director's Unit includes two special research groups focusing on advanced optics/photonics and nonlinear physics:
The Applied Photonics Group specialises in the development of novel planar and fibre light processing devices, including those with the potential for commericalisation through the Austalian Photonics Cooperative Research Centre (CRC).
The Nonlinear Physics Group is engaged in the fundamental research on the dynamics of nonlinear localised waves in various branches of physics and biophysics, including nonlinear optics, photonic crystals, condensed matter physics, and Bose-Einstein condensates.

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

Research Summary

The Director's Unit was established at the beginning of 2001, as a spin-off of the Optical Sciences Centre. It includes two special research groups, the Nonlinear Physics Group and the Applied Photonics Group, focusing on nonlinear physics and advanced optics and photonics.

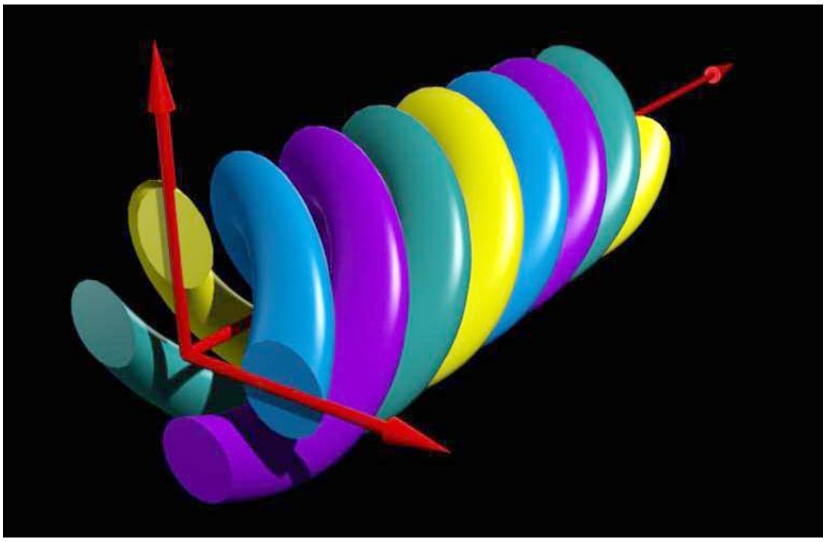
The Nonlinear Physics Group is engaged in the fundamental research on nonlinear phenomena and the dynamics of nonlinear localised waves and solitons in various branches of physics and biophysics. The interdisciplinary research of the Group covers several topics such as nonlinear effects in bulk media and optical fibres, all-optical switching devices, nano-optics and photonic crystals, self-trapping effects and energy transfer in condensed matter physics and biopolymers, nonlinear atom optics and matter waves including the dynamics of Bose-Einstein condensates.

The Applied Photonics Group specialises in the design of novel planar and fibre light-processing devices, including those with the potential for commericalisation through the Australian Photonics Cooperative Research Centre (CRC). The Group is strongly linked to experimental photonics groups within the School, across campus and within the CRC, and provides a wealth of experience and insight into the modelling and design of photonic devices and photonic integrated circuits.

Nonlinear Physics Group

During the last year, the Group was strongly supported by a grant of the Performance and Planning Fund (PPF) of the Institute of Advanced Studies and by the Australian Photonics CRC, as well as by the School. This allowed us to expand significantly in 2000 by appointing Dr Elena Ostrovskaya as a PPF Postdoctoral Fellow, and by inviting several international researchers and students for short-term visits and long-term fellowships to complement the skills and expertise of our researchers and PhD students.

2001 marked the first formal entry into the national Australian Research Council grant scheme by the School. The Group was most successful in being awarded one of the four ARC Discovery grants received by the School (Yu.S. Kivshar, Nonlinear Photonic Crystals) and, more recently, it received a second grant (C. Savage and Yu.S. Kivshar, Nonlinear Dynamics of Bose-Einstein Condensates). In addition, the Group was awarded grants by the Australia-Germany Collaborative Scheme (collaboration with the groups in Darmstadt and Münster), the Australian Academy of Sciences (collaboration with Taiwan), and by the US Air Force-Far East Research Office (collaboration with the US and Japan groups in theoretical and experimental research



A rotary cluster of four optical solitons into photonic crystal waveguides). These awards will enable the Group to extend its activities into several novel research directions such as photonic crystals and nonlinear matter waves, as well as to amplify our research in soliton physics.

The Group members continued research on optical solitons as part of an international research team composed of members of the Group and the Laser Physics Centre, working on both theory and experiment. These activities have been supported by the appointment of Dr Dragomir Neshev, a former Visiting Fellow, as a Research Fellow in a three-year position. Another Visiting Fellow of the Group, Dr Anton Desyatnikov, was awarded a Fellowship of the Humboldt Foundation and will be working with the group of our German collaborator, Professor Cornelia Denz, in Münster.

The Nonlinear Physics Group is one of the most productive research groups in Australia as measured by the number of papers published in prestigious research journals. For example, Physical Review Letters is considered as a top-ranked journal that publishes the most innovative world-class research in physics. In 2001, the Nonlinear Physics Group contributed more than 10% of all PRL papers published by Australian scientists and more than 35% of all PRL papers published by the School.

The Group plays an active role within the Institute of Advanced Studies, hosting many overseas researchers and research students. In 2001 we embarked on two new research directions, including the physics of photosensitive optical materials (in collaboration with the experimental team of Professor Satoshi Kawata from Osaka in Japan) and the field of dispersion-managed solitons in long-distance fibre communications based on the dispersion management concept (in collaboration with Chalmers Technical University, Sweden and two international research students, Andreas Johansson and Patrik Johansson).

Our interests are expanding each year, and now include areas beyond traditional nonlinear optics and soliton physics, such as linear and nonlinear propagation of light along photonic-crystal waveguides and waveguide bends, nonlinearity-induced folding and self-assembly of biopolymers, the dynamics of nonlinear matter waves, the stability of optical vortices and the dynamics of vortex matter, long-distance optical communication and all-optical switching devices. Four distinct research streams can now be identified: nonlinear optics and (spatial and temporal) optical solitons; ultra-cold atoms, matter waves and Bose-Einstein condensates; photonic crystals and waveguides (with the goal to study their nonlinear properties); and nonlinear models of biophysics. These four main directions are interlinked by our wide expertise in nonlinear physics, and the Group members share many common interests across the spectrum of nonlinear physics research.

Optical Solitons and Vortices

One of the most important research highlights of 2001 was the prediction of new phenomena in nonlinear physics – multipole multimode vector solitons – a composite optical beam in a bulk medium that can be treated as a bound state of several solitary waves, the so-called "molecule of light". This and other, complicated and intriguing objects including quadrupole vector solitons and "necklace-type" optical beams have been predicted and demonstrated experimentally (in collaboration with the Laser Physics Centre). This topic has attracted interest from other groups overseas with simultaneous experimental verifications at Princeton (USA) and Technion (Israel).

Multipole Spatial Vector Solitons

Multipole optical solitons are associated with higher-order guided modes trapped by a soliton-induced waveguide in a bulk medium. Such stationary localised waves include previously predicted vortex and dipole-mode vector solitons and also describe new higher-order vector solitons and necklace-type beams. We have developed the theoretical and experimental results of the structure, formation, and instability development of quadrupole vector solitons. (A.S. Desyatnikov, D. Neshev, E.A. Ostrovskaya and Yu.S. Kivshar; W. Krolikowski and B. Luther-Davies [LPC])

Necklace-Ring Vector Solitons

Extending the concept of multipole optical beams, we introduced novel classes of optical vector solitons that consist of incoherently coupled self-trapped "necklace" beams carrying zero, integer, and even fractional angular momentum. Because of the stabilising mutual attraction between the constituents, such stationary localised structures exhibit quasi-stable propagation over larger distances. (A. Desyatnikov and Yu.S. Kivshar)

Transverse Instability of Vector Solitons

A theory of modulational instability of multiparameter solitary waves has been developed for the first time, and was used to analyse the transverse instability of composite (or vector) optical solitons in a saturable nonlinear medium. It was demonstrated both theoretically and experimentally that a soliton stripe breaks up into an array of (2+1)-dimensional dipole-mode vector solitons, thus confirming the robust nature of those solitons as fundamental composite structures of incoherently coupled fields. [W. Krolikowski and G. McCarthy [LPC]; D.E. Pelinovsky [University of Toronto, Canada]; D. Neshev and Yu.S. Kivshar)

Dipole-Mode Vector Solitons in Anisotropic Nonlocal Self-Focusing Media

We have demonstrated, theoretically and experimentally, that dipole-mode vector solitons created in biased photorefractive media possess a number of unusual properties, such as stability of a selected orientation, wobbling, and incomplete rotation, owing to the anisotropic nonlocal response of the photorefractive nonlinearity. Such features are also associated with multipole vector solitons, and have been verified experimentally. (G.

Members of the Nonlinear Physics Group left to right: Yuri Kivshar, Anton Desyatnikov, Dragomir Neshev, Elena Ostrovskaya, Andrey Sukhorukov, Nick Robins and Tristram Alexander

McCarthy and W. Krolikowski [LPC]; D. Neshev, E.A. Ostrosvkaya and Yu.S. Kivshar)

Optical Vortices

Optical vortex-phase singularities or phase defects in electromagnetic waves constitute a unique and fascinating class of optical phenomena. They display a deep similarity to their close relatives, quantised vortices in superfluids and Bose-Einstein condensates. An invited review paper featuring the recent advances of our research on optical vortices has been published in Optics and Photonics News. (Yu.S. Kivshar and E.A. Ostrovskaya)

Nonlinear Aharonov-Bohm Scattering by Optical Vortices

Linear and nonlinear wave scattering by an optical vortex in a self-defocusing nonlinear Kerr medium has been studied analytically and numerically. In the linear case, it was found that the splitting of a plane-wave front at the vortex is proportional to its circulation, similar to what occurs in the scattered wave of an electron for the Aharonov-Bohm effect. For larger wave amplitudes, the scattering of a dark-soliton stripe (a nonlinear analog of a small-amplitude wave packet) by a vortex was studied analytically and numerically, and a significant asymmetry of the scattered wave was observed. Subsequently, a wave-front splitting of the scattered wave develops into a transverse modulational instability "unzipping" of the stripe into trains of vortices with opposite charges. (A. Nepomnyashchy [Technion, Israel]; D. Neshev and Yu.S. Kivshar)

Dispersion-Managed Solitons and their Applications

In collaboration with the research team of Chalmers University, we have investigated how to transform, with maximum efficiency, a dispersion-managed (DM) soliton into a conventional (NLS) soliton of a single-mode nonlinear optical fiber. The necessity for such analysis has been demonstrated in 1999-2000 in a number of experiments at Accatel, France, where it was shown that two DM to NLS conversions improves the efficiency of the pulse regeneration in long-haul transmission lines. We have shown that, for a wide range of the dispersion-map strength, a proper optimisation of the fiber parameters enables a large fraction of the DM soliton energy to be transferred into a fundamental soliton. Another project on robustness of the DM soliton transmission to fibre imperfections is currently underway. (A. Johansson, P. Johansson, E.A. Ostrovskaya and Yu.S. Kivshar; D. Anderson and M. Lisak [Chalmers University, Sweden])

Bose-Einstein Condensates and Atom Lasers

In the year 1999, our Group started work in a completely new and exciting field of Bose-Einstein condensation (BEC). In November 1999, in collaboration with Dr Craig Savage from the Faculties (ANU), we organised an international workshop on BEC and Atom Lasers, and hosted several visitors from Spain, New Zealand and Australia. Since then, we have initiated a number of projects in this rapidly developing area of physics. One of our first projects in this field was based on the idea of nonlinear modes of the BEC in a trap, first applied to the simplest case of a parabolic trap (Yu.S. Kivshar and T. Alexander) but then developed for the case of Josephson-like oscillations in a trap with two local minima (E.A. Ostrovskaya and Yu.S. Kivshar). Recently, the Atom Optics Laboratory in the Faculties, led by Dr J. Close, have produced the first Australian BEC which takes them a step closer to establishing a National Atom Laser Facility in future years. A number of important theoretical results have been produced in collaboration with our Group and are to be tested experimentally.

Atom-Laser Dynamics

An ideal atom laser would produce an atomic beam with highly stable flux and energy. In practice, the stability is likely to be limited by noise and nonlinear dynamical effects. The dynamics of an atom laser were investigated using a comprehensive one-dimensional, mean-field numerical model. The output beam and experimentally important effects, such as three-body recombination were modeled and it was found that at high-pump rates the latter plays a role in suppressing the high-frequency dynamics, which would otherwise limit the stability of the output beam. (N. Robins and E.A. Ostrovskaya; C. Savage [The Faculties])

Modulational Instability of Spinor Condensates

Spinor BECs, or optically trapped ultra-cold atomic clouds, are subject to parametric coupling between the spin degrees of freedom, which produce a number of interesting physical effects, some of which have already been observed experimentally. Drawing on an analogy with nonlinear optics, we have studied the modulational instability (MI) of the spinor condensates. We demonstrate, analytically and numerically, that the ferromagnetic phase of the spinor Bose-Einstein condensate may experience modulational instability of the ground state leading to a fragmentation of the spin domains (N. Robins, W. Zhang, E. Ostrovskaya and Yu.S. Kivshar). Together with other nonlinear effects in the atomic optics of ultra-cold gases (such as coherent photo-association and four-wave mixing), this effect provides a further analogy between coherent matter waves and light waves in nonlinear optics.

Atomic-Molecular Bose-Einstein Condensates

The coherent photo-association of BEC atoms and formation of Bose-condensed molecules, yet to be realised experimentally, is the matter-wave analog of second harmonic generation in nonlinear optics. We have applied some ideas and concepts of parametric optical interactions to the theory of atomic-molecular condensates (AMBEC) and successfully completed a project on the dynamics and stability of the AMBEC. We are now pursuing research on stable topological states of the AMBEC, such as ring vortices and dark solitons, and are also investigating the effects of losses on the condensate. This project is being carried out in collaboration with P. Julienne from NIST, in the USA. (T. Alexander, B. Cusack, E.A. Ostrovskaya and Yu.S. Kivshar)

Photonic Crystals and Waveguides

One of our new areas of research started last year is the study of nonlinear properties of photonic crystals and photonic crystal waveguides. Photonic crystals are usually viewed as an optical analog of semiconductors that modify the properties of light, similar to a microscopic atomic lattice that creates a semiconductor band-gap for electrons. It is believed therefore that by replacing relatively slow electrons with photons as the carriers of information, the speed and band-width of advanced communication systems will be dramatically increased, with potential benefits for the telecommunications industry. However, to employ the high-technology potential of photonic crystals, it is crucially important to achieve a dynamical tunability of their properties. This idea can be realised by changing the light intensity in nonlinear photonic crystals.

Self-Trapping and Stable Localised Modes

The existence of stable nonlinear localised modes near the band edge of a two-dimensional (2D) reduced-symmetry photonic crystal with a Kerr nonlinearity was predicted theoretically. Employing a technique based on Green's function, a physical mechanism of mode stabilisation was revealed which is associated with an effective nonlinear dispersion and long-range interaction in the photonic crystals. (S. Mingaleev and Yu.S. Kivshar)

Nonlinear Localised Waves in a Periodic Medium

The existence and stability of nonlinear localised waves in a periodic medium has been studied in the framework of the Kronig-Penney model with a nonlinear defect. The existence of a novel type of stable nonlinear band-gap localised state was demonstrated, and also revealed a generic physical mechanism of oscillatory wave instabilities associated with band-gap resonances. (A. Sukhorukov and Yu.S. Kivshar)

Parametric Localised Modes in Quadratic Nonlinear Photonic Structures

This project concerns two-colour spatially localised nonlinear modes. They are formed by parametrically coupled fundamental and second-harmonic fields excited at quadratic nonlinear interfaces embedded in a linear layered structure, i.e. a quadratic nonlinear photonic crystal. For a periodic lattice of nonlinear interfaces, an effective discrete model for the amplitudes of the fundamental and second-harmonic waves at the interfaces was derived and it was found numerically and analytically that the spatially localised solutions-discrete gap solitons can exist in such structures. For a single nonlinear interface in a linear superlattice, the properties of two-colour localised modes were studied, and both similarities to and differences from quadratic solitons in homogeneous media were described. (A. Sukhorukov and Yu.S. Kivshar; O. Bang [Technical University, Denmark]; C.M. Soukoulis [Ames Laboratories, USA])

Fourth-Harmonic Generation in 2D Nonlinear Photonic Crystals

Efficient fourth-harmonic generation in a single 2D quadratically nonlinear photonic crystal has been investigated. A novel parametric process has been proposed that starts with phase-matched generation of a pair of symmetric second-harmonic waves, which then interact to produce a fourth-harmonic wave that is collinear to the fundamental. It has been shown that this process is more efficient than conventional fourth-harmonic-generation schemes by a factor of four at low intensities, and it was also demonstrated how to design and optimise the nonlinear 2D photonic crystals that can be implemented in lithium niobate crystals. (M. de Sterke [University of Sydney]; S.M. Saltiel [Sofia University, Bulgaria]; Yu.S. Kivshar)

Nonlinear Dynamics of Biopolymers

The importance of nonlinear excitations in biology has already been emphasised in the study of biopolymers and conjugated polymers. In particular, it was suggested that nonlinear modes may provide a possible mechanism for the energy (or charge) transport and storage in proteins and conducting polymers. The concept of nonlinear localised modes was also employed to explain some specific features of DNA dynamics. The main target of this new initiative is to suggest and analyse nonlinear dynamical models that provide a relatively simple explanation for many effects known to occur in biological systems, and also the dynamics of bio-molecules. This research extends our knowledge and experience in nonlinear physics into a new venture that may produce many novel results.

Nonlinearity-Induced Conformational Dynamics of Biopolymers

Conformational flexibility is a fundamental property of polymers which differentiates them from small molecules and gives rise to their remarkable properties. A distinctive feature of biological polymers is that their elementary sub-units have a complex structure and can carry long-lived nonlinear excitations. The role of nonlinear excitations in biological functioning of proteins and DNA molecules is now being intensively studied. It is widely believed that nonlinear excitations may be responsible for storage and transport of the energy released during ATP hydrolysis. It was also suggested that the local opening of the DNA double-helix, which is necessary for reading of the genetic code during transcription, is a result of spontaneous localisation of thermal energy in the form of discrete breathers.

We have suggested a new role of nonlinear excitations in one of the most important functionalities of biopolymers, their conformational dynamics. For the first time to our knowledge, we demonstrated that nonlinear excitation may cause local softening of polymer bonds, i.e. the effective bending rigidity of a semiflexible biopolymer chain decreases in the neighbourhood of the nonlinear excitation as the amplitude of the excitation grows. When the amplitude exceeds a threshold value, the effective bending rigidity becomes negative, i.e. the nonlinear excitation, even in the absence of thermal fluctuations, causes a buckling instability of the chain. Moreover, with further growth of the nonlinear excitation amplitude, the buckling instability is replaced by a collapse instability. We described the instability analytically, and then demonstrated its role in the folding dynamics of macromolecules through 3D numerical simulations of long, semi-flexible chains. (S. Mingaleev and Yu.S. Kivshar; Y. Gaididei and P.L. Christiansen [Technical University, Denmark])

Applied Photonics Group

With the formation of the Director's Unit at the beginning of 2001, the Applied Photonics Group was established to integrate research activities that relate to the modelling and design of innovative guided wave photonic devices for telecommunications and other applications. The Group is also involved in collaborative research with experimental groups within the School, with other research groups in the Australian Photonics CRC in Sydney and Melbourne, and with various photonics companies in Australia and overseas. The outcomes of these activities include a growing number of patents, reflecting the practical importance of the research.

The Group also continues to play significant roles in presenting undergraduate photonics courses in the Science and Engineering Faculties, and in industrial education and training in photonics. This involvement was a key factor in obtaining university support of $1 million for the new ANU Photonics Degrees in both Science and Engineering that have their first intake of students in 2002. There are also key links with the Photonics Institute in Canberra, which was established by the CRC in 2001 to help promote photonics outreach, education and training at both local and national levels.

Fibre-to-Waveguide Pigtailing

A novel method for attaching buried channel waveguides to optical fibres is being developed which automatically guarantees minimum splicing loss by suitably etching the fibre and waveguide endfaces to form a plug-in-socket arrangement. This arrangement also ensures the automatic alignment of the cores of the fibre and waveguide irrespective of their alignment relative to the fibre and waveguide cross-section, respectively, and avoids the need for polishing the waveguide endface. A provisional patent has been taken out to cover the process and further developments are expected to be underwritten by a Silicon Valley company in the USA. (J.D. Love and D. Thorncraft; S. Law [University of Sydney]; S. Huntington [University of Melbourne])

Hydrogen-Free Planar Waveguides & Devices

In collaboration with the Space Plasma and Plasma Processing Group in PRL, a new range of doped silica-based materials is being developed in thin-film form using the HARE PECVD reactor. These materials are in principle H-free, which should avoid the high optical transmission loss at 1400 nm which is prevalent in existing materials due to OH-ion absorption. These materials are therefore highly suitable for the fabrication of planar waveguide processing devices that exhibit low loss over the whole available spectrum for optical communications. (J.D. Love, D. Bulla, C. Charles, W. Lei, K.W. Gaff, R. Jarvis and V. Au; R.W. Boswell [PRL])

Reduced Bend Loss in Waveguides and Fibres

With the increasing use of compact photonic integrated circuits and optical fibre-based modules for telecommunications, there is a need to reduce radiation due to tight bends in waveguides and fibres linking different parts of these circuits and modules. A novel strategy has been developed and quantified which incorporates a sophisticated design of the waveguide or fibre refractive index profile. A provisional patent has been filed covering the design and a protoype fibre is being developed in collaboration with the Optical Fibre Technology Centre at Sydney University. Interest in this fibre has been expressed by Australian industry. (S. Tomljenovic-Hanic, J.D. Love and A. Ankiewicz)

Adiabatic Light Processing Devices

There is a class of light processing devices, such as asymmetric Y-junctions, that relies on the evolution of individual modes through the device without coupling or loss of optical power. Typically in these devices, a particular mode evolves from one symmetry state into a different symmetry state relying only on the changing geometry along the device length. The rules governing the evolution of each mode have been elucidated and quantified, and used to demonstrate the practicability of a wavelength multiplexer and demultiplexer. (J.D. Love and A. Ankiewicz)

Analytical/Numerical Techniques

The determination of the fields and propagation constants of guided modes of dielectric waveguides is a classic problem in waveguide theory and has attracted much attention during the last century. Of particular interest are modes whose fields extend large distances into the cross-section from the guiding part of the waveguide, and require specialised analytical/numerical techniques. A new technique, the hybrid Fourier Decomposition Method has been developed for application to planar waveguides, where modal fields are well confined in one dimension, but can extend arbitrarily large distances in the orthogonal dimension. (S. Tomljenovic-Hanic, J.D. Love and A. Ankiewicz)

Special Optical Fibres and Tapers

There is a wide range of fibre designs and fibre tapers that have specific properties and applications. The wavelength response of a special depressed-cladding fibre has been analysed and measured experimentally in order to develop a potential application for a fibre polariser, and a multi-layered fibre has been analysed for response to sensing in fluorescing liquid samples. The effect of bending on highly tapered multimode and single-mode fibres is being quantified both theoretically and experimentally with a view to the development of very compact devices. (J.D. Love, B. Gibson and J. Katsifolis; R. Stolen [Virginia Tech University, USA])

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Professor Rob Elliman - Head of Electronic Materials Engineering

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

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

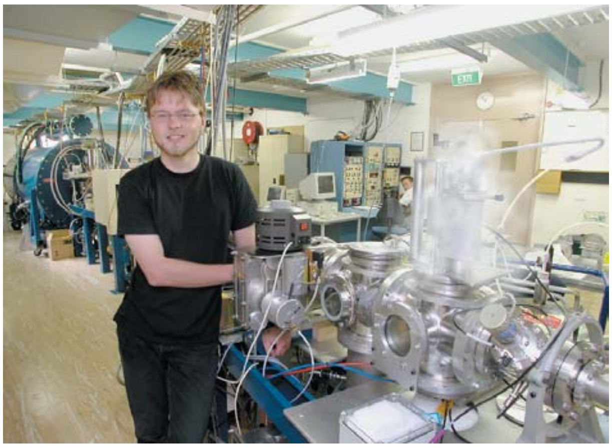
Research Summary

The research activities of the Department of Electronic Materials Engineering (EME) cover a broad spectrum of scientific and technological endeavour, ranging from curiosity-driven fundamental research to strategic, applied projects focussing on particular devices or applications. For convenience, in the research achievements listed below, the Department's research is classified into four pursuits: Ion Beam Modification of Materials; Materials Growth and Processing; Materials Analysis and Characterisation Methods; Optoelectronic Devices and Integration, reflecting its main research and equipment strengths. In reality, however, most projects straddle two or more of these pursuits and also often contain both fundamental and strategic elements.

Overall, 2001 was a highly successful but somewhat turbulent year for the Department, with entry into the ARC and efforts to launch a spin-off company, Acton Semiconductors P/L presenting new challenges. The Department was extremely successful in its first year of entry into the ARC with three grants totalling around $270,000 pa, despite only a quarter of the academic staff being eligible. The productivity and research achievements of the Department also remained impressive, with around 80 high-quality, peer-reviewed papers published in scientific journals, 10 invited or keynote presentations at national and international forums, and around 20 contributed conference presentations. In addition, the Department graduated 8 PhD students during the year, an all-time record, and continued to attract a wide range of vacation and honours students, as well as international scholars and visitors. Although the international downturn in the communications sector adversely affected progress in the Acton venture in 2001, there is optimism that significant external funding opportunities can be realised for the Department in the area of semiconductor lasers in 2002.

The range, performance and reliability of EME's research facilities continue to underpin its strong research performance. The fact that these facilities operate at peak levels and with minimum down-time is a great credit to the Department's technical staff (M. Aggett, T. Halstead, A. Hayes, B. King, D. Llewellyn and A. Watt) and technical assistants (M. Conway and A. Williams). Their expertise, commitment and professionalism are much appreciated. The crucial role played by the School's workshops and service areas is also acknowledged in this context.

There were again a number of staff and student highlights during the year. For example, C. Jagadish was elected a Fellow of the Institute of Electrical and Electronic Engineers (IEEE) and the Institute of Nanotechnology (UK), and was appointed Associate Editor of the Journal of Nanoscience and Nanotechnology; R. Elliman was promoted to level E (Professor), was elected a member of the International Advisory Committee for the "Atomic Collisions in Solids" conference series, and elected as a Member of the Governing Council of the Electronic Materials and Processing Division of the International Union of Vacuum Societies and Technical Associations; M. Ridgway was appointed to the National Scientific Advisory Committee for the new Australian Synchrotron Facility under construction at Monash University, was awarded an ARC Discovery Grant and was appointed to a standard (continuing) position in the Department; N. Fletcher was appointed an Associate Editor of the Journal of the Acoustical Society of America; N. Welham received the Rossiter W. Raymond Award of the American Institute of Mining, Metallurgical and Petroleum Engineers, and was elected to Fellowship of the Minerals Engineering Society. In addition, J. Wong-Leung was promoted from level A to level B and was awarded a QEII Fellowship and G. Azevedo was awarded an ARC Post-Doctoral Fellowship. The achievements of our students were equally impressive, with T. Weijers and S. Kucheyev receiving the AINSE Medals for the best student oral and poster presentation, respectively, at the 12th AINSE conference on Nuclear Techniques of Analysis and a Certificate of Distinction in the RSPhysSE Director's Award competition for the best student research paper; S. Kucheyev was also awarded a Graduate Student Fellowship from the IEEE Electron Devices Society and a silver medal in the Materials Research Society (MRS) graduate student competition. Adrian Cheung was awarded scholarships from both the ANU



Sergi Kucheyev in the high energy implanter lab

and the Golden Key International Honours Society. EME staff also continued their major leadership roles in professional societies such as AIP, IEEE and MRS, as well as undertaking important committee work for the University and the School.

In addition to its regular academic activities, the Department hosted two scientific meetings this year, a focussed workshop on nanotubes and fullerines in Canberra chaired by Y. Chen and the 15th International "Ion Beam Analysis" conference in Cairns chaired by R. Elliman. The honour associated with invitations to chair major international conferences, as well as the steady stream of national and international visitors (14 in 2001) who come to Canberra to collaborate with EME staff, is clear evidence of the high international regard for EME's research.

Finally, it is a great pleasure to acknowledge the contribution of our Departmental Administrator (L. Walmsley), who continued to cope with the demands of EME's staff and students, endless visitors, reports, and budgets, as well as organising conferences, managing external grants and acting as our main social organiser.

Ion Beam Modification of Materials

Optical Characterisation of Semiconductor Nanocrystals in Silica

Work has continued on the optical characterisation of semiconductor (Si and Ge) nanocrystals produced in silica by ion implantation and annealing. It has been shown that optical absorption spectra of such composite materials can easily be misinterpreted, leading to unrealistic estimates of the bandgap of nanocrystalline semiconductors and to apparent absorption bands. The bandgap error arises from scattering losses due to the $1/\lambda^4$ (Rayleigh or Mie) scattering cross-section associated with small particles. If not taken into account, this increases the apparent absorption at short wavelengths and, when plotted as a Tauc plot, leads to a greater than expected bandgap estimate. Unexpected absorption features, on the other hand, arise from interference effects associated with the depth-dependent refractive index profile produced by the implanted impurity distribution. Both effects are well known in general but have been ignored in recent work. Indeed, work in this area was stimulated by a recent report in the journal Nature of optical gain in a waveguide containing Si-nanocrystals. An absorption band attributed in this paper to a particular defect was subsequently shown to be an interference effect. Attempts to reproduce other aspects of this work were also unsuccessful, resulting in stimulated absorption rather than gain. However such measurements remain an active area of investigation. (R.G. Elliman, A. Dowd, S. Cheylan; M. Lederer and B. Luther-Davies [LPC])

Nanocrystal – Impurity Interactions

The interaction between Si-nanocrystals and impurities continues to be explored. Experiments were undertaken to further examine the effect of impurities on the luminescence intensity from Si-nanocrystals and to examine the interaction between Si-nanocrystals and rare-earth elements, such as Er. Earlier results showing that N could significantly increase the luminescence from Si-nanocrystals were confirmed and transmission electron microscopy (TEM) studies have been planned to further aid in the understanding of this effect. Preliminary studies of the nanocrystal-Er system confirmed that the 1.5 μm emission from Er could be enhanced by the presence of nanocrystals but also showed that this emission was severely compromised by radiation damage. This arose from the fact that the formation of Si-nanocrystals required annealing temperatures as high as 1100°C but the optimum annealing temperature for activation of Er is around 900°C. To accommodate these requirements, Si was implanted first and samples annealed at 1100°C to form nanocrystals. Er was then implanted and samples annealed at 900°C. However, measurements showed that the latter anneal is insufficient to completely remove the radiation damage caused by the Er implant. This led to lower than expected emission. Experiments are in progress to investigate alternative strategies. (R.G. Elliman; A. Wilkinson [FEIT]; N. Smith [Physics, Faculties]; G. Ross [IGNRS, Canada])

Panoramic view of the high energy implanter lab

Light Emission from Optically Confined Si-Nanocrystals

The confinement of light emitting material within an optical cavity of dimensions comparable to the wavelength of the emitted light can have a dramatic effect on the emission properties of the system. Such microcavities support a small number of optical modes, restricting the emission from the active medium. This results in enhanced emission at particular wavelengths and provides a method for tuning and narrowing the emission from Si-nanocrystal ensembles. In this project, microcavities containing Si-nanocrystal active layers were fabricated by plasma-enhanced chemical vapour deposition (PECVD). They consisted of a Si-rich SiO_2 layer sandwiched between wavelength selective mirrors made from alternate layers of SiO_2/SiO_xN_y. Nanocrystals were formed in the Si-rich layer by high-temperature annealing and the emission from the cavities compared with that of an isolated active layer deposited on Si. Emission from the microcavities was found to be much brighter than that from isolated layers, partly due to a narrower solid angle of emission. The emission wavelength range was also much narrower, ~20 nm fwhm compared to ~100 nm fwhm for isolated layers, and could be tuned by adjusting the thickness of the mirror layers. Exciting new results have also recently been obtained for microcavities containing a distributed active layer, in which nanocrystal-containing active layers were used as one of the Bragg mirror materials. (R.G. Elliman; T. Walsh, M. Spooner and N. Smith [Physics, Faculties])

Shrinkage of Nanocavities in Silicon under Ion Irradiation

Nanocavities are open volume defects that are stable in Si up to temperatures exceeding 900^{o}C. However, it is of both technological and fundamental interest to examine their stability under the non-equilibrium conditions of ion irradiation. In this study the interaction of irradiation-induced defects with nanocavities was examined as a function of various irradiation parameters using both in-situ and ex-situ transmission electron microscopy. Nanocavity diameter was found to decrease as a function of ion dose in both the crystalline and amorphised phases of Si and potential mechanisms for such changes have been investigated. In the crystalline phase, the decrease in diameter has been attributed to the gettering of mobile Si interstitials to the cavities during irradiation significantly above room temperature. When the Si matrix surrounding the cavities is amorphous, cavity shrinkage may be mediated by one of two processes: nanocavities can supply vacancies into the amorphous phase and/or the amorphous phase can flow plastically into the nanocavities. Both processes yield the necessary decrease in density of the amorphous phase relative to the crystalline phase of Si. The cavity diameter is also found to decrease linearly with dose at a constant temperature and this effect has only a small temperature dependence. This result suggests that the shrinkage of cavities in amorphous Si occurs when collision cascades of individual ions intersect the cavity volume. (J.S. Williams, M.C. Ridgway and M.J. Conway; X. Zhu [University of Illinois, USA]; M.-O. Ruault, F. Fortuna and H. Bernas [CNRS, France])

Ion-Beam-Induced Epitaxial Crystallisation of Si

Ion-induced crystallisation of Si can occur at temperatures much lower than thermal-only crystallisation and also offers the prospect of probing the crystallisation mechanism on an atomic scale. With such a motivation, studies of ion-beam-induced epitaxial crystallisation of amorphous Si were carried out to examine the influence of ion displacement cascades on the crystal growth rate. Detailed simulations of vacancies produced as a function of depth in various crystalline-amorphous Si structures were obtained using the Marlowe code. Results were compared with experimental growth rates for surface amorphous layers and buried layers. For the experiments, time resolved reflectivity was used to dynamically measure the extent of crystal growth as a function of amorphous layer thickness for C, Si, Ge and Au ion beams at MeV energies incident in both channelling and random crystal directions. The results indicate that Si displacements generated precisely at the interface have the dominant influence on the crystallisation process. Cascade effects with ions of different mass can have a strong influence on crystallisation rate and the rate at the surface is lower than expected, most likely as a result of oxygen knock-on effects and more dilute cascades in this region. Buried amorphous layers were also examined and large differences in growth of front and back interfaces under channelling conditions were observed. The scale of this latter effect is in reasonably good agreement with the concentration of ion-produced displacements at the interface under random and channelling conditions. (G.M. Azevedo, J.S. Williams, M.J Conway, B.C. Williams and I.M. Young; A. Kinomura [ONRI, Osaka])

Direct Observation of Voids in Ion-Irradiated Si

During ion irradiation, the forward momentum of energetic, displaced atoms causes a separation of vacancy and interstitial depth distributions. This in turn gives rise to an excess of vacancies close to the surface at depths up to about half the projected ion range ($R_p/2$) and an interstitial excess at and beyond the ion range. Whereas residual interstitial-based defects are readily observed in Si after annealing, there has been some controversy as to the stability of open volume defects in Si. In this study, the nature of residual defects in Si was examined as a function of various irradiation parameters. Under appropriate conditions, voids were clearly observed by electron microscopy and the open volume in such defects correlated with the concentration of fast diffusing metals that can be trapped at them during annealing. The results clearly show that open volume defects are stable after annealing and these defects are responsible for the trapping of metal impurities at $R_p/2$, thus explaining an observation made by many authors in recent years. (J.S. Williams, J. Wong-Leung and M.J. Conway)

Irradiation of Si with N Ions

The bombardment of semiconductor surfaces with N ions represents an interesting method to study not only the ion-induced formation of surface compounds but also the production of secondary ions, surface charging and relocation of impurities. Intense oscillations of the secondary-ion signal have been observed, which have been described by a second-order differential equation. Results indicate that they are initiated by fluctuations in nitride film thickness accompanied by fluctuations in surface charging. Segregation of impurities at a nitride-Si interface under N bombardment is much less pronounced than under O bombardment. The effectiveness of electric field as the driving force in segregation processes was studied in n- and p-type Si under N and O bombardment. For impurities which tend to become positively charged, such as Li and Na, clear differences in profile broadening have been observed between high resistivity p-type Si and low-resistivity n-type Si, indicating that electric field effects are operational due to charging of nitride and oxide surfaces during ion bombardment. Negatively-charged species, such as F, clearly show an antisegregation behaviour under O bombardment, when a stoichiometric oxide forms at the surface, but no such effect under N bombardment. (M. Petravic and P.N.K. Deenapanray)

Atomic Arrangements in Ion-Amorphised Semiconductors

Extended X-ray absorption fine structure (EXAFS) measurements continue to yield insight, at the atomic scale, of the atomic arrangement and structure in amorphised compound semiconductors. GaAs and InP have been studied extensively in both as-implanted and relaxed states. The structure of the as-implanted state does not represent the lowest energy configuration. Following thermally-induced relaxation, a reduction in structural disorder was measurable. The atomistic mechanism governing the relaxation process is now under investigation. Preliminary measurements of the structure of amorphised InAs and GaP have also commenced. Such studies will reveal whether homopolar bonding, forbidden in the crystalline phase, is a common feature in the amorphised phase of the compound semiconductors. (M.C. Ridgway and G.M. Azevedo; C.J. Glover [Lund University, Sweden]; G.J. Foran [ANSTO]; K.M. Yu [Lawrence Berkeley National Laboratory, USA])

Implantation of Radioactive Probes in Ge

The local atomic environment of implanted impurities in defective semiconductors can help determine the nature of electronic levels in the band gap of semiconductors. The perturbed angular correlation (PAC) technique has been utilised to determine the atomic environment of radioactive In probes in Ge as a function of measurement temperature and Fermi level. The measured changes in charge distribution surrounding the probe have been compared with theoretical calculations of the electric field gradients to aid in the development of a modelling code. (A.P. Byrne and N. Rao [NP]; T. Dessauvagie and R. Vianden [University of Bonn, Germany]; M.C. Ridgway, A. Khalil, D.A. Brett and G.M. Azevedo)

Disorder in Ion Implanted Group III-Nitrides

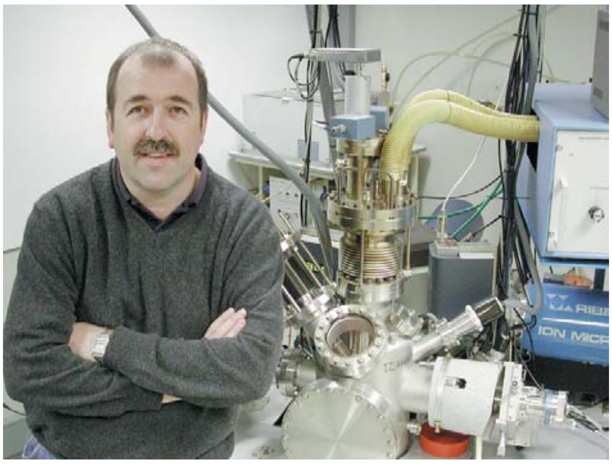
Ion implantation of group III-nitrides is a potentially important method of introducing dopants into these materials for device applications but the method suffers from the simultaneous introduction of disorder. In this study, the disorder and structural characteristics of wurtzite GaN, AlGaN and InGaN films bombarded under a wide range of implant conditions (ion mass and energy, ion dose, implantation temperature, and beam flux) have been measured. Several intriguing ion-beam-induced processes have been found, such as: (i) all materials exhibit strong dynamic annealing during irradiation, with AlGaN showing least disorder and InGaN the most disorder; (ii) preferential surface disordering, chemical and cascade density influences on damage build-up as a function of ion dose have been observed; (iii) a highly-porous amorphous GaN structure has been observed at high doses and dramatic surface dissociation has been found on annealing of such material; (iv) an enormously enhanced erosion rate is observed during some elevated temperature bombardments; and (v) blistering and exfoliation of the GaN surface can be produced following high-dose, light-ion bombardment. Such behaviour has been explained in terms of the production of mobile defects in III-nitrides even at liquid nitrogen temperatures and the separation and agglomeration of Ga and N within ion collision cascades. The quite striking structural changes, which have been observed under ion bombardment and annealing, have major implications for technological applications of implantation. (S.O. Kucheyev, J.S. Williams and C. Jagadish; J. Zou [University of Sydney]; G. Li [Ledex]; A.I. Titov [St. Petersburg State Technical University, Russia]; S.J. Pearton [University of Florida, USA])

Ion-Implanted ZnO

ZnO oxide is an interesting wide-band-gap semiconductor but has not been exploited until recently because of the poor quality of the material. However, the advent of good quality single crystals has opened up a range of potential device applications for the material and there is much interest in examining the behaviour of ZnO under typical device processing methods such as ion implantation. In this study, ion-implanted ZnO has been examined by ion channelling to study the disordering of the material. Early results have shown that defects are mobile at quite low temperatures and anomalous disorder distributions are observed in the material. (S.O. Kucheyev, J.S. Williams and C. Jagadish; J. Zou [University of Sydney])

Optical and Electrical Studies of Ion Implanted GaN

One of the applications of ion bombardment of GaN is to produce optical and electrical isolation. In this study, GaN films were bombarded under a wide range of implant conditions (ion mass and dose, implantation temperature and flux) and the changes in optical and electrical properties of the material examined by cathodoluminescence (CL) and in-situ I-V measurements, respectively. CL measurements showed that the bombardment effectively quenches band-edge luminescence but introduces other optically-active deep levels into the band gap such as so-called yellow luminescence. Detailed studies have shown that yellow luminescence arises from C impurities trapped at defect complexes and the presence of H and O can also enhance its intensity. The degree of electrical isolation has been found to depend on ion mass, ion flux and temperature as well as ion dose. The optimum value of electrical resistivity under ion bombardment can exceed 10^{11} W/sq and isolation is stable to



Mladen Petravic in the SIMS lab

temperatures of 1000^{o}C, which is ideal behaviour for device applications. However, such ultra-high resistivity values are not easy to measure and furthermore cause excessive charging effects during scanning electron microscope examination. Indeed, voltage shifts associated with such charging effects are very sensitive to the magnitude of resistivity and this behaviour can be used as a convenient way to monitor high resistivity and optimum isolation. (S.O. Kucheyev, C. Jagadish and J.S. Williams; H. Boudinov [Porto Alegre]; M. Toth [Cambridge University, UK]; M.R. Phillips [University of Technology, Sydney]; G. Li [Ledex])

Ion Implantation of SiC

Recent developments in the growth of good quality SiC epilayers have made this material a promising contender for high-power and high-frequency device applications. Ion implantation is a key processing step for the fabrication of such devices and it is important to study the dependence of ion-induced disorder on the implantation parameters. In collaboration with a Swedish group at the Royal Institute of Technology, we observed a striking dose-rate effect on implantation-induced damage accumulation in SiC. These new results give insights into the nature of annealing processes in SiC under ion irradiation. In another study, TEM examination of SiC epilayers grown with high Al doping concentrations showed an interesting second-phase formation. This study brings new information to the ternary phase diagram (Al-Si-C) that will be relevant to the understanding of equilibrium processes in SiC. (J. Wong-Leung; M.K. Linnarsson, A. Kuznetsov, M. Janson and B.G. Svensson, [Royal Institute of Technology, Sweden])

Materials Growth and Processing

MOCVD Growth of III-V Multilayers for Optoelectronics

Growth conditions on the new metalorganic chemical vapour deposition (MOCVD) reactor have been optimised on 2, 3 and 4" wafers for GaAs/AlGaAs and InGaAsP/InP material systems with excellent uniformities. The growth parameters of InGaAsP have been tuned to cover the wavelength range of 1000-1600 nm primarily for optical telecommunication applications. New designs for high-power lasers at three wavelengths of interests, 980, 1480 (for pumping of Er-doped fibre ampliers) and 14xx nm (for Raman amplification) are being grown and evaluated. Work has also been carried out to grow lattice-matched InGaP (on GaAs) for incorporation into Al-free 980 nm pump lasers. (H.H. Tan, M. Fraser, L. Fu, C. Jagadish; L.V. Dao and M. Gal [UNSW])

MOCVD Growth of InGaAsN

In the old reactor a N source, dimethylhydrazine, has been installed for the growth of the fairly new InGaAsN material. This material is of great interest due to a bowing effect with the incorporation of N that causes a shrinkage in the bandgap. Hence, by changing the In/Ga and As/N ratios, long-wavelength devices could be achieved on GaAs substrates. Futhermore, the band offset of InGaAsN quantum wells is larger than the InGaAsP quantum wells, resulting in devices that are less sensitive to temperature. Results from this study have shown that up to ~2% N can be incorporated into GaAs at low-growth temperatures. This is sufficient to shift the photoluminescence peak to 1.07 mm. However, at higher temperatures a marked improvement in the optical quality of GaAsN was observed at the expense of lower N incorporation. It was also found that post-growth annealing could improve the quality of GaAsN significantly, presumably due to annealing of grown-in defects. Deep-level transient spectroscopy (DLTS) has been used to study the electrical nature of these defects. More exciting results should unfold from this new material system as studies of structural, electrical and optical properties are underway. (Q. Gao, H.H. Tan, P.N.K. Deenapanray and C. Jagadish; B.Q. Sun and M.Gal [UNSW])

Quantum Dots grown by MOCVD

In line with various initiatives on nanotechnology, growth of quantum dots has been continued in the new MOCVD reactor by the so-called Stranski-Krastanov method. Growth parameters were studied to optimise the size and density of the quantum dots (InGaAs on GaAs). Strong luminescence has been observed from dots of 50% In content. Multiple layers of dots (stacked dots) were also grown and they provide information about the formation mechanism of the dots, the strain-induced alignment process and also the strain relaxation processes. Work is continuing to optimise the size, density and quality of dots with higher In content. The effect of post-growth annealing has also been studied. A significant blue shift, with the narrowing of the photoluminescence linewidth, has been observed. Further work will concentrate on compositional analysis of as-grown and annealed dots by TEM and electron/hole traps investigated by DLTS. Work is underway to incorporate these dots into various optoelectronic devices such as lasers and detectors. (P. Lever, H.H. Tan, P.N.K. Deenapanray, J. Wong-Leung and C. Jagadish; P. Reece and M. Gal [UNSW])

The Role of Zn Diffusion During Quantum-Well Intermixing

One of the main hurdles in the use of intermixing in device integration is the effect of Zn. Since intermixing requires an annealing step to initiate the interdiffusion process, Zn migration during the annealing could change both the electrical and optical characteristics of the devices. Work is currently progressing to address these issues. We have found that if the Zn concentration is less than ~10^{17} cm^{-3}, it will have almost no effect during the intermixing process. (M. Buda, L. Fu, J. Hay, P.N.K. Deenapanray, H.H. Tan and C. Jagadish)

Defect Engineering in GaAs

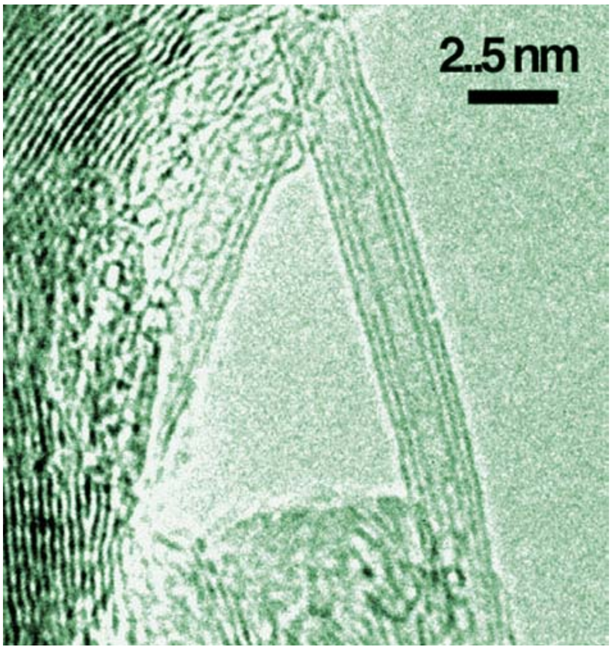
Defects play a key role in driving the disordering process in III-V semiconductors. Hence, the use of defect engineering to tailor the properties of these semiconductor materials for eventual optoelectronic device integration requires an understanding of the nature of these defects as well as their electrical and optical properties, amongst others. We have pursued our previous studies in this challenging area to devise a way to control the generation of point defects in n-type GaAs by up to two orders of magnitude using SiO_2/Si_3N_4 stacking layers. We are currently studying the segregation behaviour of impurities, such as Zn, Cu and Fe, in p-type MOCVD grown GaAs layers during the injection of Ga vacancies (i.e. impurity-free vacancy disordering). (P.N.K. Deenapanray, A. Martin, L. Fu, H.H. Tan and C. Jagadish)

C and BN Nanotubes

Studies continued on the preparation and analysis of both C and BN nanotubes. The method of preparation involved reactive ball milling to produce disordered, nanostructured material from which nanotubes could be grown, followed by annealing to nucleate and grow the tubes entirely in the solid state. The research focused on two areas: formation of large quantities of nanotubes and the mechanism of nanotube formation. A very high yield of BN nanotubes, much larger than has been achieved by other methods, has been produced by the novel ball milling method. This result clearly demonstrates that the reactive ball milling process could become a large-scale synthesis method for BN nanotubes. Multi-walled C nanotubes have also been produced by ball milling of graphite powder at room temperature and subsequent thermal annealing at 1400°C. The mechanical treatment produces a disordered and microporous structure, which provides nucleation sites for nanotubes as well as free C atoms. Multiwalled C nanotubes appear to grow from single-wall nanotube embryos via growth of the (002) layers during thermal annealing. Both C and BN nanotubes can involve metallic particles that catalyse growth but tubes also appear to be nucleated on disordered material (both BN and C) without the presence of foreign catalysts. Ceramic mills are currently being employed to try to eliminate the presence of metallic particles. [Y. Chen, J. Yu, M.J. Conway and J.S. Williams; J. FitzGerald [Research School of Earth Sciences]; L. Chadderton [AMPL])

Removal of Metals from Solar Materials

The presence of even very small concentrations of metals can seriously degrade the performance of solar cells. In this study, various methods have been investigated to remove metals from both single crystal and multicrystalline Si wafers, including the trapping of metals at heavily doped layers and at cavities. The detection and quantification of small concentrations of metals (Fe, Cr, Cu, Ag, Au, Zn and Co) was obtained by neutron activation analysis whereas recombination lifetime measurements were used to determine the effectiveness of metal gettering and removal on the solar cell properties. Known concentrations of various metals were introduced into Si wafers by ion implantation to study the effect on carrier lifetime. The effectiveness of gettering techniques to subsequently remove the metals was then examined. Results obtained provided the first quantitative measurements of the dependence of carrier lifetime on the metal concentration and enabled models to be developed to explain the behaviour. (J. Wong-Leung, J.S. Williams, K. Stewart and M. Petravic; A. Kinomura [ONRI, Osaka]; D. Macdonald and A. Cuevas [FEIT])



Electron micrograph of a BN nanotube

Mechanochemical Activation

Three major areas of work have been investigated this year and all show significant and important results for the future application of mechanical activation in radically different areas. i) Mechanochemical processing of enargite, a Cu bearing arsenosulphide mineral, has been shown to lead to substantial reaction within one hour with the formation of water-soluble copper sulphate and arsenic oxide. This route completely avoids products which are a deterrent to smelting operations and environmental problems associated with acid leaching. ii) The generally accepted method for recovering O on an extraterrestrial body is by thermal reduction of indigenous minerals, the most amenable of which is ilmenite, $FeTiO_3$. A terrestrial ilmenite has been milled for up to 400 hr and then reduced in a flowing H atmosphere. The recovery of O as water was found to be over two and a half times greater for a sample milled for 400 hr than for an unmilled sample. These highly encouraging results will be extended to simulated lunar soil and moonrock. iii) Previous work on a number of milled powders has indicated a maximum in the surface area as measured by the BET technique. Work on graphite and activated C show that this maximum is misleading and masks a major effect of milling, namely an increase in the mass of gas chemisorbed onto the surface. The fraction of gas chemisorbed onto activated C increased from 8% for unmilled powder to 70% for powder milled for 1000 hr, suggesting a novel

Panoramic view of the MOCVD lab with the new reactor (right) gas storage process, with loadings of 0.95 g gas/g of C being substantially larger than any previously reported. (N.J. Welham)

Material Analysis and Characterisation Methods

Surface Roughening in SIMS by O and N Ions

Surface roughening of Si under energetic ion bombardment can degrade the depth resolution in secondary ion mass spectrometry (SIMS) profiling. The effects of roughening have become increasingly important in the profiling of ultra-shallow junctions in semiconductors. The influence of surface roughening on SIMS depth resolution has been studied in Si. AFM was used to examine the roughening of SIMS craters obtained by O- and N-beam bombardment at different angles of incidence. A correlation has been found between the critical angle for compound formation and the enhanced roughening of the crater bottoms. (P.N.K. Deenapanray and M. Petravic)

High-Resolution Photoemission from Hydrogenated Semiconductor Surfaces

Studies continued on the application of synchrotron radiation in the analysis of semiconductor surfaces by measuring the high-resolution photoemission from hydrogenated GaAs surfaces around Ga 3d and As 3d levels. GaAs (100), (110) and (111) surfaces were examined by photons in the 40-160 eV range from the beam-line 08A LSGM at the Synchrotron Radiation Research Center (SRRC) in Hsinchu, Taiwan. Chemical shifts in Ga and As levels were monitored as a function of H exposure. From the chemical shifts, information on H bonding sites was obtained. For example, on the polar GaAs (100) surface, for low exposure (1×10^4 L of H_2), H atoms bond preferentially to As, as demonstrated by the chemical shift of the As 3d level but no shift in the Ga 3d level. (M. Petravic, P.N.K. Deenapanray; J.-M. Chen [SRRC, Taiwan])

Selective Photodesorption from Semiconductor Surfaces

Resonant core-level ionisation by photon irradiation is known to be chemically selective. Studies continued on the selective removal of H from hydrogenated GaAs surfaces of different orientations by photon irradiation from the beam-line 08A LSGM at SRRC. Selectivity in desorption of H atoms has been demonstrated from As or Ga atomic sites on GaAs surfaces by tuning the photon energy to specific core-level energies of Ga and As. (M. Petravic, P.N.K. Deenapanray; J.-M.Chen [SRRC, Taiwan])

Bonding Arrangements for Metals Trapped at Cavities in Si

The trapping of fast diffusing metals at defects in Si (gettering) is a topic of considerable technological interest. In this study, atomistic metallic-impurity gettering mechanisms in Si have been identified with a variety of characterisation techniques including Rutherford Backscattering (RBS), EXAFS and PAC. The efficiency of nanocavities as gettering sites for Pd impurities has been measured as a function of implantation dose and annealing temperature. EXAFS and PAC measurements have been correlated in an attempt to identify the gettering sites and reconstruction processes for Cu, Au and Pd impurities on nanocavity inner surfaces. Furthermore, PAC measurements of Pd-dopant complexes have commenced to deduce the proposed pairing mechanism and results have been correlated with measurements of minority-carrier lifetime. (M.C. Ridgway, G.M. Azevedo, D.A. Brett, A. Khalil; A.P. Byrne and N. Rao [NP]; A. Cueves and D. Macdonald [FEIT])

Pulse-Height Discrepancies in High-Energy Heavy-Ion Detectors

Work has continued on the response of both gas-ionisation and Si surface-barrier detectors to high-energy heavy-ions. For gas ionisation detectors the measured pulse height for high-energy heavy ions was found to be significantly less than that for light ions of the same energy. This pulse-height deficit has been studied in some detail and can be partially accounted for by the increased fraction of energy lost in the detector window and in nuclear scattering processes for heavy ions. However, a substantial component of the deficit remains unexplained. Recent experiments suggest that it may result from electron-ion recombination in the high-density ionisation track of the heavy ions and experiments have been planned to test this model. Work on Si surface-barrier detectors has also continued and showed for the first time a complex dependence of e, the energy required to create a detectable electron-hole pair, on the ion mass. In particular, it was shown that e first decreased and then increased with increasing ion mass, so that a pulse-height surplus was recorded for masses up to 80 amu and a pulse-height deficit for higher masses. This has important implications for precision measurements using surface-barrier detectors and further studies of the underlying mechanisms are in progress. (T.D.M. Weijers and R.G. Elliman; H. Timmers [ADFA]; J.A. Davies [McMasters University, Canada])

Energy Loss and Straggling of High-Energy Heavy Ions

Measurements of heavy-ion energy loss and straggling data are required for many applications, including quantitative ion-beam analysis. Unfortunately, the accuracy of such data is currently limited to ±20%, imposing limits on the accuracy of techniques such as heavy-ion elastic-recoil analysis and heavy-ion backscattering spectrometry, and preventing accurate assessment of newly developed theoretical models. In an ongoing collaborative study with the University of Lund and the University of Newcastle, measurements of the stopping power and straggling of a range of heavy ions have been undertaken

Fu Lan in the electrical testing laboratory for energies around 1 MeV/amu. Recent measurements have concentrated on the stopping of Si ions in Si targets, covering the energy range 0.1–0.7 MeV/nucleon. (R.G. Elliman and T.D.M. Weijers; H. Timmers [ADFA]; H. Whitlow [University of Lund, Sweden]; D.J. O'Connor [University of Newcastle])

Heavy-Ion Elastic Recoil Detection Analysis of Materials

The unique capabilities of the heavy-ion elastic recoil detection (HI-ERD) technique continue to be developed and exploited for a range of collaborative studies involving the quantitative detection of a broad range of elements, including H. Such analysis has been aided by the DataFurnace program that has been customised for analysis of our data and by the use of an experimental Monte Carlo computer code, that is capable of simulating spectra including such effects as plural and multiple scattering. (R.G. Elliman and T.D.M. Weijers; H. Timmers [ADFA])

Nanoindentation of Semiconductors

There has been considerable recent interest in contact-induced deformation modes of semiconductors, partly as a result of the requirements of the semiconductor industry but also driven by strong fundamental questions about pressure-induced phase transformations and other unusual structural changes that could arise during indentation. In this study, nanoindentation has been undertaken in a range of semiconductor substrates to examine deformation mechanisms in detail. The approach has been to correlate the mechanical behaviour of these materials with structural changes, including phase transformations, as monitored by several methods including in-situ electrical measurements. Results have led to the first comprehensive reports on the evolution of deformation with increasing pressure in Si, Ge, GaAs, InP, GaN and ZnO. Catastrophic plastic deformation, mediated by either slip or phase transformation depending on the material and the loading conditions, has been observed. In Si, a transformation to a metallic phase has been monitored by electrical measurements. It is possible to observe the precise onset of such a transformation with increasing load and how this material responds on unloading. Deformation mechanisms have been proposed for all these materials. ZnO is a particularly interesting material since it is extremely soft in comparison with the other semiconductors studied and contact-induced defects are observed to propagate well beyond the stress fields under the indenter. (J.E. Bradby, J.S. Williams, J. Wong-Leung and S.O. Kucheyev; M.W. Swain [U. of Sydney]; P. Munroe [UNSW])

Optoelectronic Devices and Integration

980 nm High-Power Laser Diodes

Optimisation of kink-free, high-power 980 nm pump laser diodes was done using a non-conventional asymmetric laser diode structure. The COD (catastrophical optical damage) output power is 200 mW per facet for uncoated facets and the best device shows kink-free operation up to 150 mW per facet (300 mW both facets). Special asymmetric structures, such as thin p-clad (d = 0.3 um) and low divergence (16∞ FWHM) structures with very low absorption factor, operating at 980 nm, were also designed, fabricated and characterised. (M. Buda, J. Hay, L. Fu, H.H. Tan, C. Jagadish and J. Lalita)

Ultrafast Photodetectors

Ion implantation of InP for ultrafast photodetector applications has been continued with the work extending to In, P, Ga and As implants. Strain introduced by ion implantation has been found to be different in the case of In with respect to other ions. Transmission electron microscopy studies were carried out to study the changes in defect structure after ion implantation. These changes in structural properties are correlated with the optical and electrical properties. [C. Carmody, H.H. Tan, M. Buda and C. Jagadish; M.J. Lederer, V. Kolev and B. Luther-Davies [LPC]; L.V. Dao and M. Gal [UNSW]; J. Zou [University of Sydney])

Saturable Absorber Mirrors

Further collaboration with the Laser Physics Centre concentrated on the design, growth and ion implantation of semiconductor saturable absorber mirrors with large absorption to fabricate mode-locked 1064 nm solid-state lasers with even faster response time and larger modulation depth. (H.H. Tan and C. Jagadish; V. Kolev, M. Lederer and B. Luther-Davies [LPC])

Integration of a Diode Laser and a Waveguide

The technique of intermixing was applied to the fabrication of integrated optoelectronic devices. We have successfully integrated a laser diode with a 2.5 mm waveguide region. The device characteristics are very promising, with a internal loss in the passive waveguide region of only 7 cm^{-1} and very little degradation in the laser section. (M. Buda, L. Fu, H.H. Tan and C. Jagadish)

Impurity-Free Vacancy Disordering for Integrated Optics

Further work has been carried out on controlling the impurity-free vacancy disordering (IFVD) process to establish its suitability for device integration. The effect of P and Ga dopants in spin-on glass (SOG) films on IFVD in (In)GaAs/AlGaAs quantum well (QW) structures was investigated. It was found that P-doped SOG films created a similar amount of intermixing as that of undoped SOG films but by varying the concentration of P, the amount of intermixing could be controlled. On the other hand, samples with Ga-doped SOG layers showed suppression of intermixing, opening up the possibility of using it as a cap/mask for suppressing intermixing. Parallel to this, changing either the O content of a PECVD oxide layer or its deposition rate could control the extent of intermixing. In other related work, different dielectric caps, such as PECVD SiO_2, Si_3N_4 and SOG were deposited on the GaAs/AlGaAs QWs followed by a further deposition on top of these dielectric caps. Significant suppression of interdiffusion was also observed. A two-step mechanism, which includes the generation of Ga vacancies as well as their diffusion under the influence of the stress field in the QW structure has been proposed to explain this observation. Results indicate that Ga_xO_y may also be used as a mask material in conjunction with other dielectric capping layers in order to suppress IFVD. Both methods look promising in achieving selective area intermixing in optoelectronic device integration by IFVD. (L. Fu, P.N.K. Deenapanray, J. Wong-Leung, H.H. Tan and C. Jagadish)

Other Areas

Acoustics Research

Collaborations have continued with a variety of researchers on the topic of acoustics that is separate to the major materials programs in the Department. The main emphasis of this work has been in musical and biological acoustics. All the projects have led to significant publications during the year. Collaboration with ADFA in the area of aeroacoustics, the interaction of moving objects with air to create sound, involved the study of various forms of vibrating reed valves and also the production of sound by the Aboriginal "bullroarer". Another Aboriginal instrument investigated in collaboration with Melbourne University and UNSW is the didjeridu, and the UNSW collaboration has also produced research results on flutes. All of these projects have been supported by various ARC Large Grants. Studies of the vibration of solid structures, involving CSIRO, have been extended to the investigation of the vibration of fractal objects such as hyperhelices. An experimental and theoretical study of the re-voicing of the National Carillon in Canberra has also been undertaken. Research of a more industrial nature on the design of condenser microphones has continued with CSIRO, NAL and a commercial partner. Finally, bioacoustics research has continued with a number of Australian and international colleagues. (N.H. Fletcher; A.Z. Tarnopolsky and J.C.S. Lai [ADFA]; J. Wolfe and J. Smith [UNSW]; T. Tarnopolskaya and F.R. De Hoog [CSIRO]; W.J. Bailey [University of WA]; H.C. Bennet-Clark [Oxford, UK])

Staff

Professor and Head of Department
Rob Elliman, BAppSci, MAppSci RMIT, PhD DSc Salf, FAIP (from August)
C. Jagadish, BSc MSc (Tech) MPhil PhD, FAIP, FIP, FIoN, FIEEE (until August)

Professor and Associate Director (Resources, RSPhysSE)
Jim Williams, BSc PhD NSW, FAIP, FIEAust, FTSE

Professor
C. Jagadish, BSc MSc (Tech) MPhil PhD, FAIP, FIP, FIoN, FIEEE (from August)

Senior Fellows
Rob Elliman, BAppSci, MAppSci RMIT, PhD DSc Salf, FAIP (until July)
Mark Ridgway, BSc McM, MSc PhD Queen's

Fellows
Ying Chen, BSc CAS MSc Tsinghua, PhD Paris (ARC Fellowship, jointly with FEIT)
Mladen Petravic, MSc Zagreb, PhD

ARC QEII Fellow
Hoe Tan, BE Melb, PhD (from June)

Research Fellows
Manuela Buda, PhD Eindhoven
Hoe Tan, BE Melb, PhD (until May)
Heiko Timmers, Dipl.Phys. Munich, PhD (ARC Fellowship, jointly with Nuclear Physics) (until July)
Jenny Wong-Leung, BSc Bristol, PhD (ARC Fellowship) (from July)

Postdoctoral Fellows
Gustavo de Medeiros Azevedo, DSc Universidade Federal do Rio Grande do Sul (CNPq Fellowship, Brazil)
Sanju Deenapanray, BE PhD
Jenny Wong-Leung, BSc Bristol, PhD (ARC Fellowship) (until June)

Visiting Fellows
Henri Boudinov, BSc MSc PhD Sofia (until January)
Richard Brown, PhD Melb
Stuart Campbell, BSc Aberd, MSc Salf, PhD Mon, FAIP
Suk-Ho Choi, BS Seoul, MS PhD KAIST
Paul Edwards, BSc PhD Tas, FAIP, FRAS, FIREEAust, FIEAust, FNZEI. SMIEEE
Neville Fletcher, MA PhD Harv, DSc Syd, FIP, FAIP, FAAS, FTSE, FAA, AM
Lalita Josyula, M.Phil Delhi, PhD Stockholm
Atsushi Kinomura, PhD Osaka
Jeff McCallum, BSc PhD Melb
Bengt Svensson, MSc Goth, PhD Chalm Tech (until January)
Nick Welham, BEng Leeds, PhD Lond DIC, FMES
Joachim Wolter, PhD Marburg/Lahn

Research Assistants
David Llewellyn, (joint with Electron Microscopy Unit, RSBS)
Tony Watt, AssocDipSci Inst Bdgo CAE, BApplSci Swinburne

Head Technical Officer
Tom Halstead, ElectCommCert Canb TAFE

Senior Technical Officers
Michael Aggett, AssocDipMechEng CIT
Alan Hayes, AssocDipMechEng CIT
Bernie King, ONC UK

Laboratory Technicians
Martin Conway
Antony Williams

Departmental Administrator
Laura Walmsley

Laser Physics Centre

Professor Barry Luther-Davies - Head of Laser Physics Centre

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

http://laserspark.anu.edu.au

Research Summary

Much of the research within the Centre involves some aspect of materials science where there have been a number of exciting developments this year. These include the discovery of a paramagnetic carbon nano-foam produced by pulsed laser deposition; demonstration of electrochemical switching of the cubic nonlinearity in organometallic molecules; and the commercialisation of organically modified glasses (ORMOSILs) developed in the Centre with support from the Australian Photonics Cooperative Research Centre. This last development has involved the transfer of ANU-developed IP to a new start-up company Redfern Polymer Optics (RPO) which was established late in 2000 as the newest member of the Sydney-based Redfern Photonics group of companies. RPO aims to sell optical integrated circuits fabricated using ORMOSIL glasses to the telecommunications market. The company has established clean room and device fabrication facilities within the Innovations Building at the ANU and a number of RPO staff have been appointed as Visiting Fellows to the Centre. These include Dr Dax Kukulj, Dr Robbie Charters, Dr Graham Atkins and Dr Congji Zha (who transferred to RPO from a CRC funded post in September). Dr Weitang Li also joined the Centre with his time shared between the RPO project and the HARE project within the Plasma Research Laboratory.

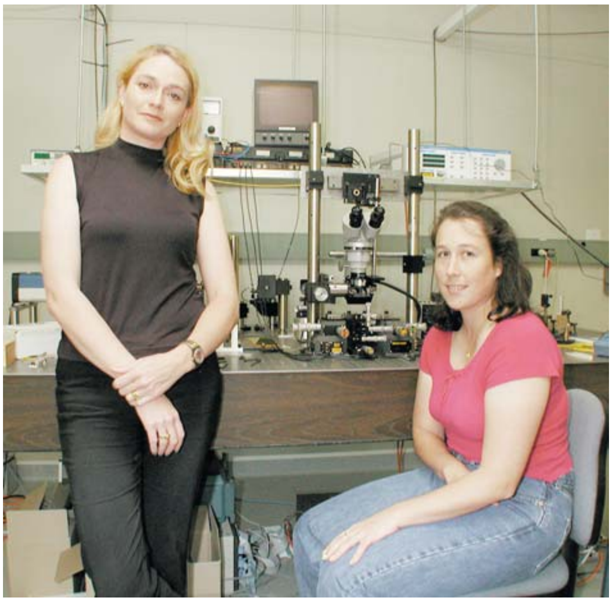
The Centre remains an important contributor to the research of the Australian Photonics CRC and Professor Barry Luther-Davies holds positions as CRC Research Director, is a member of the CRC Executive and is a Director of Australian Photonics Pty Ltd, the Commercial and Management agent for the CRC. Other CRC supported projects include a novel scheme for spectral analysis of RF data using four dimensional holography; the application of pulsed laser deposition technology to the production of waveguide films in chalcogenide glasses; work on optical spatial solitons and non-linear optical materials; and a project fully-funded by ABB and Transgrid to develop a voltage sensor based on a polymer optical fibre. The research of the CRC in micro- and nano-technology was presented by Professor Luther-Davies at Nanotechnology Workshops in Japan and Korea attended by an Australian delegation and arranged by DISR. Follow up visits have so far involved representatives from LG Elite in Korea and AIST in Japan.

The Centre was pleased to have three of its staff promoted this year. Neil Manson was rewarded for his exceptional contributions to solid-state laser spectroscopy by promotion to Professor. Dr Ken Baldwin who heads our programs in VUV Laser Spectroscopy

Staff associated with RPO Pty Ltd

and is a major contributor to the Atom Manipulation project carried out in collaboration with AMPL was promoted to Senior Fellow. Dr Max Lederer, who oversees our work on the development of novel short pulse lasers, was promoted to Research Fellow.

We welcomed a number of new staff and students during the year. In addition to those involved in the RPO project, Dr Olivier Uteza joined us in June with support from an IREX Fellowship to work with Dr Andrei Rode. Dr Anna Samoc was reappointed for a further five year period. Ms Lily Luo joined us as a technical assistant working on the industry-funded Polymer Optical Fibre project replacing Therese Martin. Cindy Bradley stepped in as Departmental Administrator until September whilst Kristina Milas was on sick leave. Five students joined the Centre: Elliot Fraval, Jevon Longell, Syed Queddes, Yinlan Ruan and Eleni Notaras who was also a recipient of a Redfern Photonics Scholarship. Bronwyn Taylor worked in the Centre as a vacation scholar on laser ablation of dental tissue and has subsequently become a regular student visitor as part of a collaboration with Macquarie University on the development of Ytterbium mode-locked lasers. Ben Cornish undertook a project as part of his final year Engineering degree and also a period of work experience.



Sam Ashby and Ruth Jarvis in the device testing lab

Research Accomplishments

Nonlinear Optical (NLO) Materials and Structures

Following the upgrade last year of our experimental facilities, we are now able to perform NLO measurements with high power 100 femtosecond duration laser pulses across the full range of wavelengths from 500-2000 nm. We have used this new facility to study various classes of materials including conjugated polymers, organometallic molecules, chalcogenide glasses, metal clusters and metal-glass interfaces. Our materials work involves collaboration with many groups including Professor Rob Elliman in the Department of Electronic Materials Engineering; Dr Mark Humphrey from the Department of Chemistry, The Faculties, ANU; Professor H. Hoerhold's group at the University of Jena; and Dr Wong's group from the Baptist University of Hong Kong. A highlight of this year's research has been the discovery of reversible electrochemical switching of the cubic nonlinearity in certain organometallic structures.

Our work on spatial optical solitons continues to attract much attention with a focus this year on vector solitons including stable multi-pole structures.

Third-Order Nonlinear Properties of Model Molecules and Polymers

A large number of model molecules, oligomers, dendrimers and polymers have been studied. This included a novel conjugated copolymer of polyphenylenevinylene and triphenylamine (TPA-PPV) synthesised in Professor Hoerhold's laboratory in Germany. TPA-PPV (which is also of interest because of its electroluminescent properties) offers good processability and enhanced non-linear properties.

We have found (in collaboration with Dr Humphrey's group at the ANU) that some organometallic Ruthenium complexes, of linear, octopolar and dendrimeric type possess high values of two-photon absorption cross sections (σ_2). Interestingly, dendrimeric structures appear to provide some advantage for obtaining high values of both the refractive and absorptive nonlinearity. Our recent development is an organometallic molecule with $\sigma_2 \approx 3000 \times 10^{-50}$ cm^4/s which has the highest σ_2/M (M= molecular weight) ratio reported so far for an organometallic.

Soluble oligomers of poly(p-phenylenevinylene) synthesised by Dr Wong's group in Hong Kong exhibit large nonlinearities, increasing with the length of the conjugated chain. They also show strong wavelength dispersion effects manifested by a change of sign of the real part of the molecular hyperpolarisability. An unexpected and yet unexplained phenomenon is the sensitivity of the sign of the refractive nonlinearity to the solvent environment in which the NLO measurements are performed. A similar effect has already been observed for another class of oligomeric compounds: oligovanillines. (A. Samoc, M. Samoc and B. Luther-Davies; M.G. Humphrey and coworkers [Chemistry, Faculties]; M.S. Wong and coworkers [Baptist University, Hong Kong] and H.H. Hoerhold and coworkers [Jena University, Germany])

Electrochemical Switching of the Cubic Nonlinearity in Organometallics

We have discovered a new effect in organometallics containing oxidisable metal centres which causes switching and hence control of the third order non-linear optical properties of the material. Little is known about switching third-order NLO response, although any change in the structure of a molecule such as induced by light, should result in the change of the cubic hyperpolarisability.

Here we studied the effect of electrochromic switching in Ru acetylides on the third-order non-linear optical response by using in-situ femtosecond Z-scan at 800 nm. Three sample molecules: an octopolar π-conjugated complex; a linear analogue; and a relatively small complex with low nonlinearity were measured. In all three cases the transfer of an electron from the oxidisable Ru atom led to the creation of a molecule showing strong saturable absorption at 800 nm. Electrochromic switching, therefore, led to reversal in sign of both the absorptive and the refractive parts of the cubic nonlinearity. This observation has some interesting implications and could lead to photonic devices whose non-linear properties can be switched electrically. (M. Samoc, B. Luther-Davies, M.G. Humphrey and M. Cifuentes [Chemistry, Faculties]; G. Heath and coworkers [Research School of Chemistry])

Second-Order Nonlinear Optical Materials

An efficient route for synthesis of highly-soluble unsymmetrical oligo(phenylenevinylenes) (OPVs) for use as electro-optic chromophores in a PMMA host has been developed. The OPVs are end-substituted with donor alkoxy and acceptor sulfonyl groups for charge polarisation and incorporate a methacrylate unit suitable for copolymerisation with methylmethacrylate (MMA). The newly developed synthesis, which involved utilising an unsymmetrical precursor, methyl 4-(bromomethyl)benzoate proceeded via several straightforward and high-yield steps using the Wittig-Horner reaction to form all trans-configured OPV derivatives at high yields.

Replacement of the n-decyl chain utilised in work last year by a 2-ethylhexyl group results in vastly increased solubility of the oligo-PPV derivatives in MMA allowing these new monomers to be used for the preparation of homogeneous high-quality NLO chromophore-containing poly-methylmethacrylate films and fibres.

The second-order non-linear optical properties of the monomer and polymers were investigated by electric field poling of doped PMMA films. Comparing the signals due to second harmonic generation with those from a film of disperse red (DR1) side chain polymer, provided a relative value of the hyperpolarisability $(\mu\beta)_0 = 0.67$ in agreement with model calculations.

In cooperation with Redfern Polymer Optics a new dual functionalised type of azo chromophore with high non-linear optical activity has been synthesised. The silane group attached at one side of the molecule will allow the chromophore to be incorporated into a inorganic polymer glass (IPG), whereas the methacrylate unit can be polymerised during poling, which gives a highly oriented chromophore stable against de-poling. (A. Freydank, E. Notaras and M. Samoc; M. Humphrey Dept. of Chemistry, ANU])

Soliton Physics

In collaboration with our colleagues in the Nonlinear Physics Group within the Director's Unit we have continued to study both experimentally and theoretically, phenomena associated with the creation and interaction of optical spatial solitons. We have produced the first experimental demonstrations of multi-component, multi-pole (dipole, quadrupole, and hexapole) spatial solitons in self-focusing photorefractive medium. We have also observed experimentally the transverse instability of the two-component stripe soliton leading to formation of an array of dipole-mode vector solitons.

On the theory front we have developed an exact solution to the problem of bright and dark one-dimensional solitons propagating in a weakly non-local non-linear medium as well as a rigorous proof of the absence of collapse of 2D beams in a non-local Kerr-like medium. (W. Krolikowski; D. Neshev, E. Ostrovskaya and Yu S. Kivshar [DU])

Photonic Materials and Devices

Organic Waveguides for Photonics

We are involved in a project to commercialise organically-modified silicate glasses that were developed with support from the Australian Photonics CRC for the production of planar optical waveguide devices. Commercialisation is being carried out by a start-up company, Redfern Polymer Optics, with ANU and CRC staff contracted as consultants.

Organically modified silicate glasses (ORMOSILs) for integrated optical and opto-electronic devices have been synthesised by sol-gel processing of functionalised alkoxysilanes. Process parameters were optimised to achieve highly reproducible low cost materials which possess low optical loss in the NIR range (0.3 dB/cm @ 1310 nm and 0.6 dB/cm @ 1550 nm) and show good photo-sensitivity for pattern production. Promising routes to lower optical losses and new processing methods for ORMOSIL glasses have been identified.

We have developed the expertise to create patternable metal surface electrodes on our ORMOSIL materials for control of the resulting optical devices. As part of an Honours project carried out by Engineering student Ben Cornish, we completed a study of the residual photosensitivity of fully processed ORMOSIL films to assess their use for writing Bragg gratings. An automated grating characterisation system was developed as part of the project. The material photosensitivity was characterised using facilities at the Optical Fibre Technology Centre at the University of Sydney and the Centre for Lasers and Applications at Macquarie University. (R. Friedrich, C. Zha, G. Atkins, D. Kukulj, W. Li, R. Charters, B. Luther-Davies, R. Jarvis and B. Cornish)

Polymer Fibre for Voltage Sensing

The work, funded by ABB and Transgrid, aims to develop a single-mode polymer optical fibre voltage sensor for the power industry. We have continued to work on the fabrication of polymer optical fibre (POF) preforms capable of yielding single-mode optical fibre – a task that has proven to be unexpectedly challenging. In addition we have developed new routes (reported above) for synthesising an electro-optic chromophore for incorporation into the core of the fibres.

The fibre preforms consist of plastic rods synthesised by radical polymerisation of acrylates, and contain core and cladding parts. The second-order non-linear optical chromophore was successfully attached as a side chain to the PMMA main chain by bulk co-polymerisation with methylmethacrylate, benzylmethacrylate (BMA) and ethylacrylate. Highly transparent material has been obtained using various preform manufacturing processes. A POF fibre with a relatively low optical loss in the visible spectral range, of the order of a few dB/m at 780 nm, was recently drawn although this fibre was two moded at 1550 nm indicating a reduction in core size is still required. (A. Samoc, T. Martin, X. (Lily) Luo, A. Freydank, R.M. Krolikowska, C. McLeod, J. Bottega, B. Luther-Davies and M. Samoc)

Laser/Matter Interaction Physics

Laser Deposition of Chalcogenide Glass Films

We continued to develop our patented ultra-fast laser ablation process for the creation of waveguide films with high optical nonlinearity using chalcogenide glasses. This year 3-5 μm thick As_2S_3 films were deposited by ablating bulk glass samples using the second harmonic of a mode-locked Coherent Antares Nd:YAG laser (λ = 532 nm, t_p = 50 ps). Up to 7 W of second harmonic output was available at 76 MHz (pulse energy ~80 nJ).

The films created in this way showed improved photo-sensitivity in the as-deposited state compared with those produced last year using a Q-switched mode-locked laser. This allowed direct writing of single-mode waveguides using a computer-controlled laser writing system. The surface quality of the deposited films was exceptional with RMS roughness of the order of 0.4 nm over the 15x15 μm^2 area in 5 μm thick films. Waveguide losses as low as 0.2 dB/cm at 1550 nm in laser-written waveguides were measured. By coating the As_2S_3 with PMMA it was found that the intensities that could be used for laser writing could be increased approximately 100 fold relative to the uncoated films, allowing writing speeds of 16 mm/s to be achieved. This markedly reduced the production time for low-loss waveguides.

As part of our program to develop pulsed laser ablation for the production of low-loss non-linear waveguides, we have started to characterise the non-linear optical properties of a number of chalcogenide glasses. We have recently completed measurements of Gallium Lanthanum Sulphide (GLS) bulk glass that was fabricated in the Centre by Anita Smith. The nonlinearity was found to be two orders of magnitude higher than silica at 1550 nm making it a promising material for an all-optical processor. We have also obtained samples of $As_{24}S_{38}Se_{38}$ glass from the group headed by Kathleen Richardson at the University of Central Florida. This glass is expected to have an even higher optical nonlinearity although some of its physical properties are inferior to those of GLS.

In order to take advantage of the unique properties of ultra-fast pulsed laser ablation in materials research, we have begun to construct an upgraded experimental facility. We have started construction of a new vacuum chamber for laser deposition for chalcogenide films in particular and have designed a new 100-W 10-ps “slow” mode-locked laser as the ablation source. This installation will not only allow new materials and thin films to be created, but will also match industry specifications in terms of deposition rate, stoichiometry of the deposited films, surface quality and thickness homogeneity over large areas. (A.V. Rode, M. Samoc, R. Charters, B. Luther-Davies, Y. Ruan and A. Smith)

Electronic and Magnetic Properties of Carbon Nanofoam produced by Ultra-Fast Pulsed Laser Ablation

A new form of carbon material, a low-density cluster-assembled carbon nanofoam has been produced by high-repetition-rate laser ablation of a glassy carbon target in an ambient non-reactive Ar atmosphere. The carbon nanofoam is remarkable for many reasons. It displays high electrical resistivity and noticeable rigidity combined with extremely low bulk density.

Close inspection of all the data obtained (DC-conductivity, optical absorption, transmission and electron microscopy, electron energy loss spectroscopy) has led to the following microstructural model. There appear to be segregation of sp^2-bonding and sp^3-bonding domains, with the latter located predominantly at the surface of the approximately 60 Å sized foam clusters, and the former confined within the clusters. The sp^3-bonding between the clusters accounts for the observed low conductivity of the foam. We note that this arrangement of the sp^2- and sp^3-bonding in the individual cluster is the reverse of that observed recently in the core of so-called carbon ‘onions’, or nested fullerenes.

Electron spin resonance (ESR) measurements have shown a number of unusual features, with the main result of a very large concentration of unpaired spins of approximately one unpaired spin per 60 atoms. The high density of spins leads to paramagnetic susceptibility of the foam, which is in a striking contrast to diamagnetic properties of all other known allotropes of C. The foam contains no paramagnetic impurities at concentrations high enough to provide this spin density. Therefore, we hypothesise that these spins are due to under-bonded C atoms acting as free radicals within the clusters. The significant paramagnetic susceptibility of the carbon nanofoam arises as a consequence of its structure. (A.V. Rode and B. Luther-Davies; E.G. Gamaly, A.G. Christy and S.T. Hyde [AM]; R.G. Elliman [EME]; A.I. Veinger [Ioffee Physical-Technical Institute, Russia])

Intensity-Dependent Transient Reflectivity of Gallium during the Phase Transition induced by Femtosecond Laser

The transient reflectivity of thin gallium films induced by the femtosecond laser pulse has been studied by the pump-probe technique at different pump intensities. The time-resolved reflectivity rise rate of the femtosecond probe strongly depends on the pump beam intensity. We demonstrate that the transient electron-phonon collision rate extracted from the reflectivity data is a strong function of the temperature (laser intensity), which is drastically different from the rate observed in the equilibrium conditions. The scenario for the microscopic kinetics of the phase transition on the femtosecond time scale is proposed and discussed. New experiments for observation of time-resolved optical properties with two simultaneous identical probes are in progress. (A.V. Rode, M. Samoc, B. Luther-Davies and O. Uteza)

Sub-Picosecond Laser Ablation of Dental Enamel

Since the first use of lasers in the medical field, the contact-free application of laser light for removal of hard dental tissue has been studied as a means for replacing conventional surgical tools. To date, lasers have not succeeded in replacing the dental drill in many hard tissue applications due to slow material removal rates and unacceptable collateral damage. For conventional pulsed-laser ablation with pulses from 100 ps to microseconds, a strong thermal shock wave is accompanied by cracking of the remaining bulk material and inefficient, uncontrolled material removal. However, in recent years the development of high-average-power, high-repetition-rate sub-picosecond lasers is causing a rebirth of interest in laser surgical applications due to precise and highly effective ablation capabilities with minimal thermal and shock-wave collateral damage. We applied femtosecond laser ablation for removal of hard dental tissue with the aim of finding the laser characteristics required for replacing conventional surgical tools.

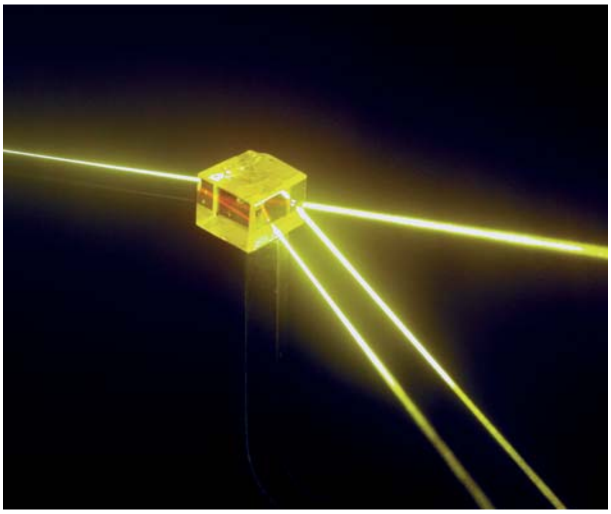
As part of a project undertaken by vacation student Bronwyn Taylor from Macquarie University, laser ablation of dental enamel has been studied over the intensity range (0.1-1.4)x10^{14} W/cm^2 using 95 fs and 150 fs pulses at a pulse repetition rate of 1 kHz. The experimentally-determined ablation threshold of 2.2±0.1 J/cm^2 was in good agreement with the theoretical predictions based on an electrostatic ablation model. The absence of collateral damage was observed using optical and scanning electron microscopy. Pulpal temperature measurements showed an increase of about 10°C during the 200 s course of ablation. However, air cooling with a rate of 5 l/min resulted in the intrapulpal temperature being maintained below the pulpal damage threshold of 5.5°C. The material removal rates for sub-picosecond precision laser ablation of dental enamel are comparable with other techniques. (A.V. Rode, E.G. Gamaly and B. Luther-Davies; B.T. Taylor and J. Dawes [Macquarie University]; A. Chan [Private dental practice]; R.M. Lowe and P. Hannaford [Swinburne University of Technology])

Electrostatic Mechanism of Ablation of Solids by Femtosecond Lasers: Ablation Thresholds for Metals and Dielectrics and Ion Acceleration

The electrostatic mechanism of ablation of solids by intense femtosecond laser pulses has been described in an explicit analytical form. It was shown that at high intensities when the ionisation of the target material is completed before the end of the pulse, the ablation mechanism is the same for both metals and dielectrics. The physics of this new ablation regime involves ion acceleration in the electrostatic field caused by charge separation created by energetic electrons escaping from the target. The formulae for ablation thresholds and ablation rates for metals and dielectrics, combining the laser and target parameters, were derived and compared to experimental data. The calculated dependence of the ablation thresholds on the pulse duration was in agreement with the experimental data in a femtosecond range, and it was linked to the dependence for nanosecond pulses. E. Gamaly [AM]; A.V. Rode and B. Luther-Davies; V.T. Tikhonchuk [University of Bordeaux, France])

Ultrafast Semiconductor Spectroscopy, Semiconductor Saturable Absorbers

We have refined our apparatus for ultra-fast pump-probe spectroscopy of semiconductors so that it can be used at all wavelengths of interest, spanning from the visible to the near infrared, and with pulses as short as 10 fs. In collaboration with EME we have continued our work on design, manufacture and characterisation of ion-implanted semiconductor saturable absorbers. Recent successes were the semiconductor saturable absorber mirrors (SESAMs) designed for solid-state laser mode-locking at 1040 nm. Using ion-implantation we have tailored the devices for use in laser crystals such as the novel Yb:YAB for which the short response times of ion-implanted SESAMs are indispensable. We are also currently working on the femtosecond differential reflectivity characterisation of ion-implanted InP. Finally, we are investigating beryllium doping of ion-implanted GaAs (collaboration with Professor U. Keller, ETH Zurich) as a promising method to increase the non-linear modulation of ultrafast ion-implanted GaAs devices. (M. Lederer, V. Kolev and B. Luther-Davies; H. Tan, C. Carmody and C. Jagadish [EME]; M. Haiml and U. Keller [ETH Zurich, Switzerland])



Rare Earth doped silicate crystal used for quantum computing

Passively Mode-Locked Ultrashort-Pulse Solid-State Lasers

In collaboration with Macquarie University and using our ion-implanted SESAMs, we have mode-locked the novel self-doubling laser crystal Yb:YAB, for the first time, producing sub 200 fs pulses at an average power of 440 mW. We have developed a number of other SESAM mode locked lasers included a high efficiency Nd:YLF system operating at 1053 nm and an ultra-low repetition rate (3.1 MHz) SESAM mode-locked high-power diode pumped Nd:YVO_4 laser for use in pulsed laser ablation experiments. The laser has the lowest repetition rate to date of any mode-locked laser.

In collaboration with the University of Karlsruhe, Germany, we have designed novel broadband ZnTe/ZnSe/CaF_2 output coupling mirrors for use with ultra-short pulse lasers and fabricated them using electron beam evaporation. These have proved to be key components in experiments that led to the first demonstration of sub 5 fs pulses with an octave-spanning spectra generated in a Kerr-lens mode-locked Ti:Sapphire laser. (M. Lederer, V. Kolev, A. Boiko and B. Luther-Davies; H. Tan and C. Jagadish [EME]; B. Taylor and J. Dawes [Macquarie University, Sydney]; R. Ell, U. Morgner and F.X. Kaertner [University of Karlsruhe, Germany])

Solid-State Laser Spectroscopy

The Solid-State Laser Spectroscopy Group's primary concern is with the understanding and the application of quantum coherence effects in solids. These range from coherence of electronic/nuclear spin levels with application for quantum computing to coherence effects in optical transitions with application to RF and microwave signal analysis.

In all cases the coherence is detected optically and relies on a range of high-resolution lasers. The prime example is an actively frequency-stabilised tunable dye laser which has a stability of better than 100 Hz. In the past year a series of actively stabilised external tunable diode laser systems have been developed with a short-term stability of 1 kHz. These lasers operate near 1.5 μm and are aimed at applications which can use components developed for telecommunications purposes such as a 40 GHz modulator.

The two groups of materials of interest are rare-earth or ion doped crystals and colour centres in diamonds. The common feature of the two materials is long spin coherence times and the ability to monitor and manipulate the spins using optical techniques. The studies of these systems have been focussed on a better understanding of the statics and dynamics of the spin levels in the ground and optical excited state.

Rare-Earth Optical Computing

There is a growing interest in rare-earth ion doped crystals for quantum information processing as a practical alternative to atomic systems. Much of this interest stems from the long coherence times of both the optical and nuclear/electronic spin transitions. The long coherence times are reflected in the narrow homogeneous line widths which we have observed to be as small as 100 Hz for the optical transitions and 5 Hz for the nuclear spin transitions.

Currently work is being carried out to determine the feasibility of a quantum computer architecture developed within the group. The architecture, based on the optical manipulation of nuclear spins, promises to be extremely robust and flexible whilst at the same time avoiding the need for complex fabrication techniques. The feasibility study is concentrating on Eu and Pr doped Y_2SiO_5. The first step concluded this year has been to fully characterise the wave-functions involved to determine transition frequencies and probabilities for all the hyperfine transitions. This was achieved using Raman heterodyne NMR measurements as a function of magnetic field strength and orientation. This data has been fitted to obtain accurate values for the ground and excited state Hamiltonians.

Aside from providing insight into quantum computing, work on these rare earth systems is expected to lead to impressive demonstrations of electromagnetic-induced transparency, slow light and trapped light.

Mechanisms that limit the coherence times of the spin transitions and techniques for suppressing them are also being investigated. These studies have already led to almost a ten-fold increase in the spin coherence time over what is reported in the literature.

The final aspect of the feasibility study is the characterisation of the interactions between the dopant ions. (J. Longdell, E. Fraval, M.J. Sellars and N.B. Manson)

Optical Processing

The long coherence times of rare-earth impurity ions in solids can be utilised in other ways. For example, the coherence established by short light pulses applied within the coherence time of typically 1 ms interfere with one another and give rise to a frequency grating in the ground and excited state. In the case of hole-burning material, this grating can remain for many hours and when the material is excited with a single short light pulse will regenerate the original pulse sequence. Thus the pulse sequence is stored. The technique, termed time domain optical memory, has been studied in the Centre over a numbers of years. The difference from the conventional approach is that by using the highly stable laser and an interferometer the entire light waveform can be reconstructed – amplitude and phase. The interferometer has also been simplified by providing a reference beam, which passes through the sample co-linear with the data and signal pulses. This provides a powerful and flexible phase-sensitive time domain memory scheme.

Data storage and recovery is an example of simple optical processing. However, the approach is more attractive for advanced processing which takes advantage of the large bandwidth and time-bandwidth product. A case in point is the development of a radio/microwave frequency spectrum analyser, a project funded by DSTO and the Australian Photonics CRC. The unique feature of this device will be its ability to perform real-time spectrum analysis, monitoring of all frequency channels all of the time. In this application a grating is stored in a hole-burning material and used to scatter a beam modulated by the unknown radio frequency. The time dependence of the output indicates the frequency of the radio frequency field. The operating wavelength was chosen to be 1.54 μm corresponding to an absorption line in Er-doped Y_2SiO_5 and enables us to capitalise on the communication technology available in this region. A 16 MHz bandwidth, 50 kHz resolution prototype has been demonstrated. In principle, the analyser bandwidth is limited by the inhomogeneous width of the infrared transition, which is currently ≈1 GHz. Efforts are underway to increase this to 100 GHz by developing modified crystal growth techniques. (D. Scott, M.J. Sellars and N.B. Manson)

Electromagnetically-Induced Transparency

The nitrogen-vacancy centre in diamond has proven invaluable for the study of strongly driven transitions and has been studied over a number of years. Transitions within the nuclear and electron spin levels are studied using a novel optical/RF three-wave mixing scheme where a resonant laser and RF field create a stimulated optical field. The stimulated beam is detected as a heterodyne beat with the magnitude proportional to the coherence of the spin system. This provides the means of studying coherence in the spin levels and the technique can be optimised by working close to an anti-crossing of the electron spin levels. There is also a fortuitous optical pumping of the population into a single spin state which enhances the signal such that they are obtained with excellent signal to noise. The nitrogen-vacancy centre has been used in this way for studies of driven two and three level systems. In the present year we have studied the case where a three-level system is driven by two strong fields and probed by a weak field. Experiment and theory have covered both the homogeneously broadened and inhomogenously broadened situations.

The nitrogen-vacancy centre has also been used to study electromagnetically induced transparency. This is where the application of a field resonant with one transition can reduce the absorption of a field resonant with a second transition. Such studies have been made in many laboratories world wide. However, the aspect of our work that has not been covered elsewhere is the situation where the transparency is perturbed by the application of a further electromagnetic field. In our case there are six spin levels and only three are involved in regular electromagnetically-induced transparency. There are then various ways other fields can be applied and it is found that they can destroy, shift or split the sharp transparency feature. A specific cased modelled through the year is where there is an apparent interaction between an electromagnetically-induced transparency and a spectral hole. There is a splitting of the electromagnetically-induced feature and this is explained satisfactorily. (E.A. Wilson and N.B. Manson)

Spectroscopy and Crystal Growing

The spectroscopy of the nitrogen-vacancy centre in diamond used in the studies of driven two-level and three-level systems and electromagnetically-induced transparency is not well understood. However, in the current year we have been able to explain the optical pumping cycle and show that with a centre perfectly aligned with an external magnetic field it was possible to have the optical cycling pump the population into a single nuclear hyperfine level. This creates a Boltzman-type distribution which would normally require cooling to mK or lower. Although this aspect is now understood there are concerns over the ionisation state of the centre under optical excitation and this is being investigated.

The studies of up-conversion and lasing in Er-doped $KYLiF_5$ have been concluded in the year. This was done in collaboration with Professor Brain Henderson, Cambridge University, UK and Professor Ann Silversmith, Hamilton College, NY, USA

There has been preliminary operation of the crystal growing furnace for preparation of double doped Y_2SiO_5 material. These crystals are required for enhanced performance of the time domain spectrum analyser. (A. Smith, M.J. Sellars and N.B. Manson)

Atom Manipulation

The atom manipulation project is a joint program between the Laser Physics Centre and the Atomic and Molecular Physics Laboratories (AMPL) which uses laser cooling and trapping techniques to investigate applications of atom optical elements to new devices on nanometre scales, and to study fundamental atomic collision physics (see AMPL annual report).

The Atom Manipulation Project has a "bright" ($>10^{10}$ atoms/second) beam line source of laser-cooled metastable He atoms which is used to investigate new atom optical elements that manipulate the atomic de Broglie wave. This facility is being used to study, for example, the guiding of atoms through hollow optical fibres using evanescent light fields. A similar metastable He source facility is used to generate liquid nitrogen-cooled atoms for applications such as atom lithography, where this year we have been developing an apparatus to study the relative contributions of UV light and several metastable atomic species to the lithography process.

This year has also seen the implementation of a third beam facility based on a liquid helium-cooled, metastable He source. By operating this source at liquid helium temperatures (~5 K), we have generated an atomic beam with velocities of several hundred m/s. Already the cryogenic source has shown promise for focusing the atomic beam using transverse molasses, due to the

LPC students with the high resolution laser system and crystal structure models long interaction time that the slower source allows. Using this beam, we hope to avoid the need for large scale Zeeman slowing in order to load our metastable helium magneto-optical trap for experiments with ultracold atoms. (R. Dall, V. Leung, J. Swansson and K.G.H. Baldwin; S.J. Buckman [AMPL])

UV Laser Spectroscopy

In parallel with the finalisation of the near-continuum (175 nm) spectrum of the oxygen Schumann-Runge band system (see AMPL annual report), work has continued on a joint project with Macquarie University to develop new high-resolution laser spectroscopic sources. This year we have injected cw radiation at 1.5 mm from an external cavity diode laser (ECDL) developed at ANU into an optical parametric oscillator (OPO) constructed at Macquarie that is pumped by a 1.06 mm Nd:YAG laser. The next stage is to construct a similar OPO based on a periodically poled KTP crystal injected with 842 nm light from a further ECDL system, which may ultimately be applied to improve precision measurements of the helium 1S – 2S transition. (K.G.H. Baldwin; M. Kono [AMPL]; Y. He, R. White and B.J. Orr [Macquarie University])

As part of a collaborative program with the Vrije (Free) University of Amsterdam, Dr Ken Baldwin undertook a series of experiments this year using the XUV laser facility at the VU. The aim was to study the $b^1\Pi_u$ state of diatomic nitrogen, whose predissociation rate is a key input for the photochemical processes in terrestrial and planetary atmospheres. The XUV laser facility employs narrowband UV (frequency doubled visible) radiation which is frequency tripled in a pulsed Xenon jet to allow 1 + 1 (XUV + UV) ionisation spectroscopy that is single (XUV) photon resonant with the $b^1\Pi_u$ state.

This work studied the ro-vibronically resolved electronic spectra up to v = 9 in the isotopes $^{14}N_2$, $^{14}N^{15}N$, and $^{15}N_2$. This data measured the less abundant isotopic spectra for a number of these bands for the first time, and extends previous measurements for known bands to higher J. The data yielded both the isotope shifts and the predissociation lifetime for the $b^1\Pi_u$ state of the isotopomers, providing new information to allow further development in the UV Physics Unit (AMPL) of models for the molecular potentials. (K.G.H. Baldwin; J.P. Sprengers and W. Ubachs [Vrije University of Amsterdam, Netherlands])

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Maryla Krolikowska
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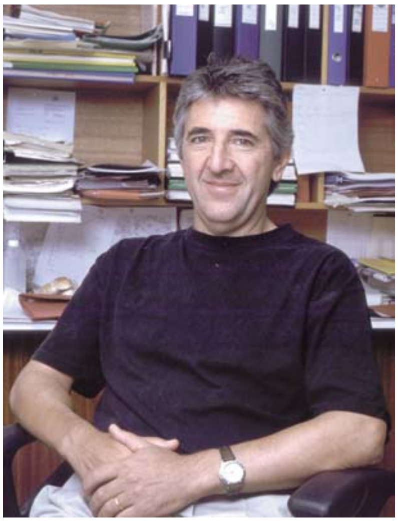
Cindy Bradley (until September)
Kristina Milas (from September)

Nuclear Physics



Professor George Dracoulis - Head of Nuclear Physics

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

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

Research Summary

Fundamental studies of the nucleus are aimed at elucidating its unusual properties which derive from its quantal, many-body nature. The nucleus is unusual in that while it contains only relatively few particles, it can exhibit both single particle and collective properties from competing motions. These are often delicately balanced in that the characteristic states are at comparable excitation energies and in regions of low-level density such that they can interfere and mix. The study of such properties in nuclei, which can be produced under a variety of conditions using heavy-ion reactions is the main aim of nuclear spectroscopy. The wide range of complex interactions which occur between the colliding nuclei themselves is the subject of nuclear-reaction-dynamics studies. In spectroscopy, different reactions are chosen to produce nuclei that are usually not found in nature, whereas in reaction studies, the target and projectile, and the collision conditions, may be chosen to investigate the coupling of the relative motion to the internal, nuclear, degrees of freedom. Since nuclei of different internal structure can be used, 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 opportunities that arise to apply new accelerator and detection techniques to benefit other areas of science, the research program is continually being developed. It currently includes:

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

Success in many activities relies heavily on the ability of the 14UD electrostatic accelerator to provide nuclear beams of a range of masses, precisely defined in energy and time. These characteristics are the basis of comprehensive studies of both nuclear structure and nuclear dynamics. The accelerator itself, and many of the techniques and instruments developed for basic research are also used in high-sensitivity applications. This year has again seen consistent activity in all research areas, using a wide variety of beams. Incremental progress has been made in developing the Linac booster to deliver beams of higher energy and higher mass than is available with the 14UD alone, to all experimental stations. This includes a program of re-plating of resonators with the aim of increasing the high-field limits, and a restructuring of the beam optics to improve beam intensities.

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

In order to maintain international competitiveness, at the same time as providing facilities for other users, continuing attention must be paid to detector instrumentation and accelerator and ion-source technology. Recent enhancements of the research capabilities which affect the accessibility of the facility to outside users include a more flexible data-acquisition system capable of handling larger multiple-element high-resolution detector arrays and the concomitant high count rates. The system is now in general use. In the fission-fusion area, first beams have been delivered into the new fusion product separator SOLITAIRE based on a superconducting solenoid, and full commissioning is imminent. The majority of funding for both of the above projects was won through earlier bids to the ARC Research Infrastructure, Equipment and Facilities (RIEF) schemes. In the spectroscopy area, augmentation of the γ-ray array CAESAR, which is the central tool of the spectroscopy pursuit, is also in progress with funding support from the University Major Equipment Committee. Supplementary funding because of currency fluctuations has been sought, and completion of the project which will bring much higher efficiencies, is now anticipated for early to mid 2001. In the area of Nuclear Moments and Hyperfine Fields, components of the new instrumentation funded through a RIEF grant last year are being assembled. The aim of this project is to enhance our capabilities for the study of electric and magnetic fields surrounding atomic nuclei in solids. The activities of the Accelerator Mass Spectrometry group have been expanded with new staff funded from the School's successful bid to the Institute Planning Committee. This will allow a new emphasis on research related to environmental studies.

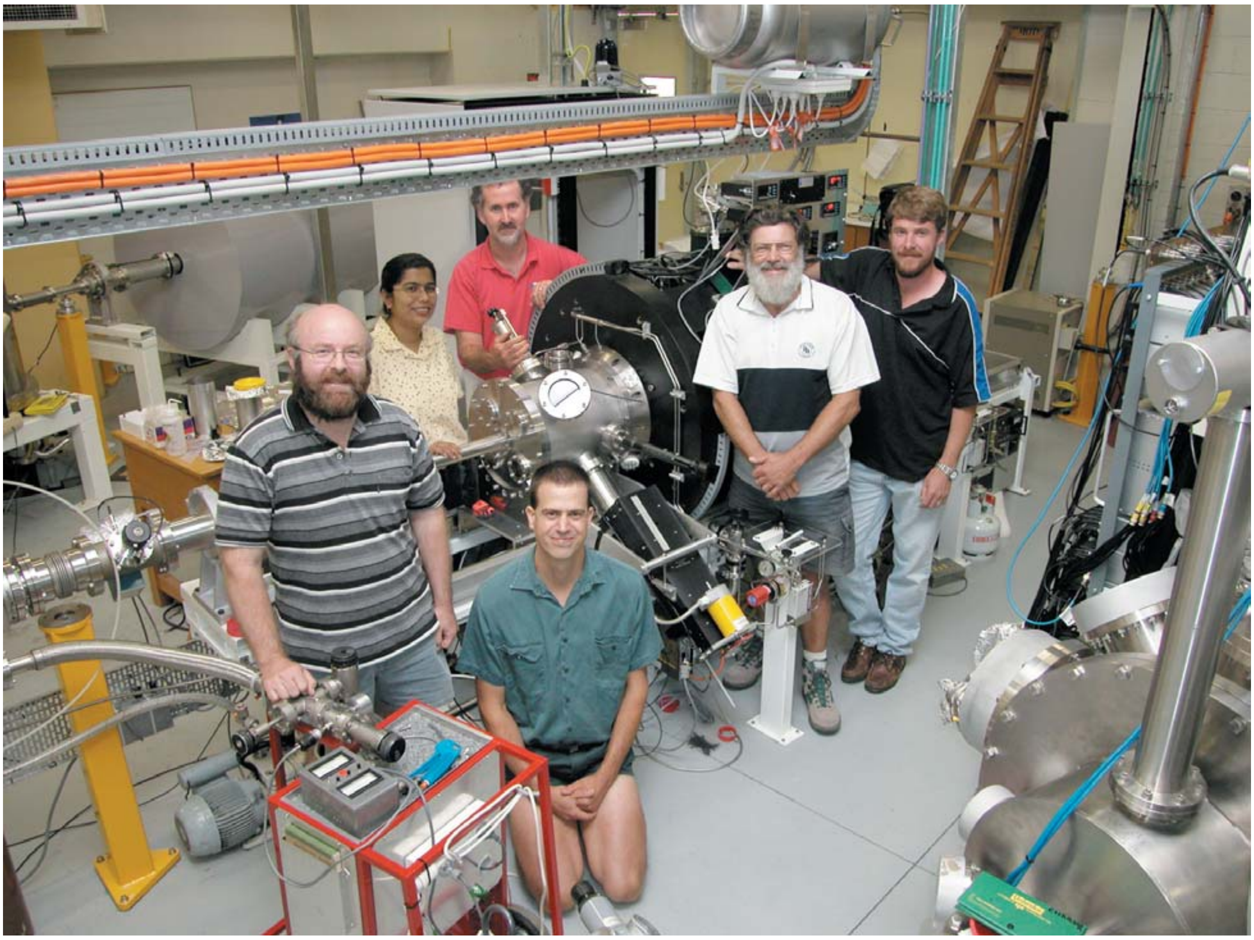
Staff changes in the AMS group included the resignation of Paul Hausladen to continue his Postdoctoral Fellowship at Oak Ridge National Laboratory, the appointment of Vladimir Levchenko as a Research Officer, Tim Barrows as a Postdoctoral Fellow and Lukas Wacker as a Postdoctoral Fellow (one year). Mariana di Tada from Buenos Aires who was a long-term visitor in AMS has returned to Argentina and Guaciara dos Santos who was a Visiting Postdoctoral Fellow supported by CNPq has returned to Brazil. Paul Davidson who re-joined the Department for a short period to work on the Data Acquisition project has now been appointed to a position as a Research Officer, to provide computing support for the Department and accelerator users. Robert Bark of the Nuclear Spectroscopy group was promoted to Fellow, and Greg Lane and Anna Wilson joined the group as Research Fellows. Igor Gontchar has joined the Fission/Fusion group for one year, while Heiko Timmers (ERDA) who held a joint appointment between Nuclear Physics and EME as an ARC Fellow was appointed to a lectureship at the Australian Defence Force Academy. Heiko intends to continue collaborations with both departments. New Visiting Fellows also include Allan Baxter (all the way from the Faculties) working with the Spectroscopy group, as is Chang-Bum Moon from Hoseo University who has been funded by the Korean Research Foundation. Narayanan Rao from Sao Paolo has joined the PAC experimental group with support from FAPESP (Brazil).

Restructuring of the Accelerator building to meet the needs of users for detector development and testing and sample preparation for AMS is now in progress and will continue through the early part of 2002, with funding from the University's Capital Management Plan.

More details of all aspects of the Department's activities and research studies, some of which are sketched out below, are available in the Department Annual Report for 2001 (ANU-P/1501), available on request, and on the Department web page http://wwwrsphysse.anu.edu.au/nuclear/.

Fusion and Fission Dynamics with Heavy Ions

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



The new SOLITAIRE fusion product seperator and some of the design team

The activities of the group are focused on elucidating the dynamical processes of nuclear fusion and fission, two of the most important reactions in nuclear physics.

The understanding of the influence of the fusion configuration on the subsequent evolution of the combined system, leading either to a combined heavier element via fusion, or to fission, with no heavy product, is vital to predicting reactions which will allow formation of superheavy elements. The PhD thesis work of Annette Berriman, who studied three reactions forming ^{216}Ra, with different mass projectiles, has shed light on the interplay of fusion and fission, with implications for superheavy element formation. Part of this work was published as a letter to Nature this year. (This article won for Annette the Director's prize for the best student paper of the year.)

Further studies of this type in the Department will be facilitated by the new superconducting solenoid fusion product separator SOLITAIRE. Following its delivery last year, this year has seen the construction and installation of the upstream target vacuum chamber and the downstream detector chamber, together with the complex gas handling system. Successful first beam tests were carried out.

Another development of infrastructure to aid in interpretation of experimental data is the completion of a computer code to calculate exactly fission-fragment angular distributions as part of Rachel Butt's PhD project. These are the first calculations ever to take into account all spin effects that influence fission angular distributions, and exotic angular distributions in fission following fusion of deformed nuclei with large ground state spin have been predicted.

Experimental work this year involved exploiting the breakthroughs developed during the ^{216}Ra work, through extension of the energy range of the data using the Linac, and investigations with a wider range of projectiles, in reactions forming ^{215}Fr. Investigations of the breakup of weakly bound nuclei continued to build a consistent picture, showing that breakup significantly affects fusion in reactions on heavy nuclei. A measurement of fusion of ^{12}C with ^{6}Li, using a ^{12}C beam, to give higher-energy fusion products, showed conclusively that there is no evidence for suppression of complete fusion in this reaction. On the contrary, completion of the analysis of the extensive data set for ^{6}Li + ^{209}Bi confirmed the dramatic suppression of complete fusion, yields being only 63% of those expected, and with concomitant large yields of incomplete fusion products. A new approach to analysis of sub-barrier breakup promises to throw light on the relationship between this phenomenon and the suppression of complete fusion at above-barrier energies. (A.C. Berriman, R.D. Butt, M. Dasgupta, I.I. Gontchar, D.J. Hinde, C.R. Morton, A. Mukherjee and J.O. Newton)

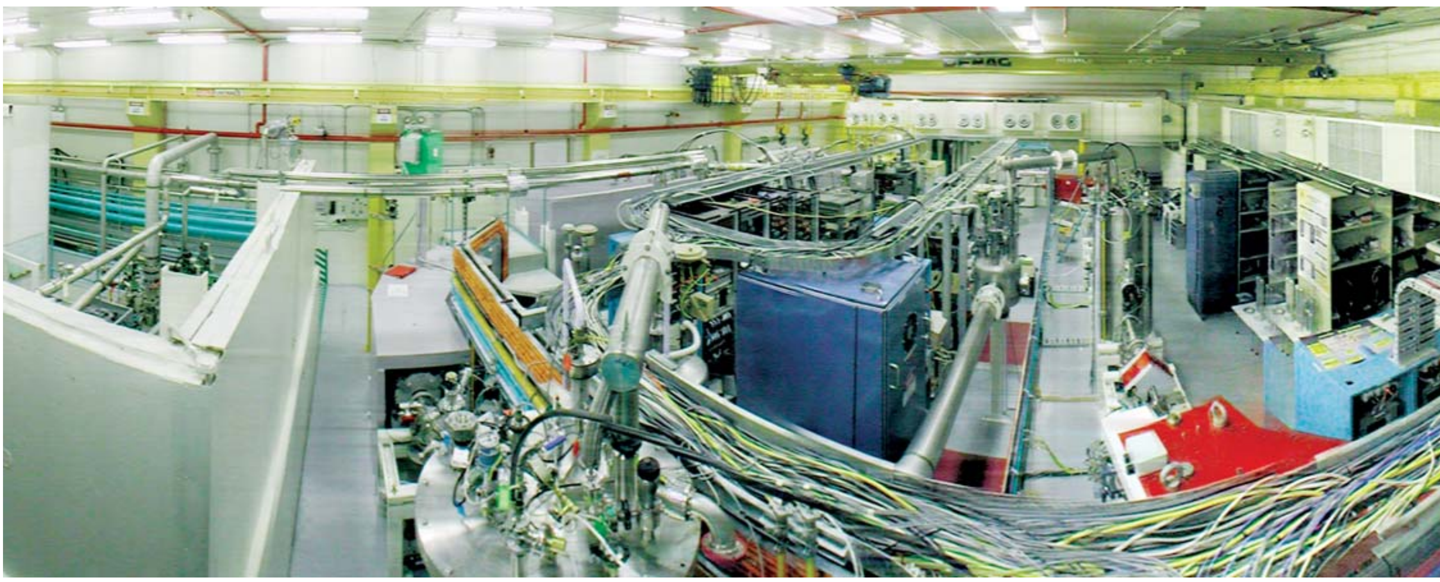
Nuclear Spectroscopy

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 studies of multi-quasiparticle intrinsic states in deformed nuclei, not far from stability, have continued with evaluation of results on the lutetium isotopes from a series of experiments in the last few years, now complete. One of the main results has been the observation of local mixing effects which result in abnormally fast transitions from high-K states. In collaboration with UK groups, we have continued studies of high-K isomers in the odd and odd-odd rhenium iotopes resulting in the identification and characterisation of new multi-quasiparticle isomers whose properties are being compared with the predictions of model calculations.

Previous work on the osmium isotope ^{184}Os carried out in collaboration with the UK groups has also come to fruition with the establishment of a comprehensive level scheme. A feature of the scheme is the large number of intrinsic levels at high spin which are apparently of high-K, but which have very short lifetimes, indicative of triaxiality and shape fluctuations. Studies of the neighbouring nucleus ^{185}Os have been instituted to attempt to map the trend to increasing triaxiality oberved in ^{186}Os and heavier isotopes.

Although no new measurements have been carried out, we have also put forward an interpretation of recent measurements by other groups of the inelastic photon scattering on ^{180m}Ta. It is the only naturally occurring isomer, being found in its 9^{-} excited



Panoramic view of the LinAc booster hall state, rather than the shorter-lived ground state, and its production in nucleosynthesis, and survival is the subject of some controversy. We have shown that the lowest observed photon resonances which result in the eventual de-excitation of the isomer, a process which would have profound implications for the survival of ^{180m}Ta in the stellar environment, match excited states identified in our earlier comprehensive spectroscopic studies. This association is the first concrete identification of candidates for such intermediate states. A consistent analysis of the decay widths confirms that the E1 strengths are abnormally large, a possible consequence of statistical K-mixing in regions of high-level density.

In a different region where the nuclei are soft and very susceptible to triaxial deformations, the main focus has continued to be the measurement and analysis of rotational bands in nuclei which might show evidence for predicted chiral (or aplanar) rotation modes. A candidate has been observed in ^{134}La and several other odd-odd nuclei have been studied in detail.

Our other major area of interest is the studies of shape co-existence, particularly in the region of the very neutron-deficient lead isotopes. Using a combination of electron measurements for multipolarity measurements and γ-γ-time coincidence studies with pulsed beams, we have successfully resolved anomalies in the decays from the 11^- yrast state in ^{192}Pb and shown that the abnormally enhanced E3 decays, which are also seen in ^{190}Pb and in a range of neutron-deficient polonium isotopes, may all have the same origin, specifically an effect of hybridisation induced by an oblate deformation. This provides subtle evidence for the co-existence of different shapes in these nuclei. On a similar theme, analysis of our measurements carried out using Gammasphere at the Lawrence Berkeley National Laboratory which were aimed at characterising the isomeric states observed in our earlier work on ^{188}Pb, is nearing completion and is showing evidence that supports the contention that the isomers are all of different character, and representative of three different deformations. Those results have been supplemented by electron measurements using SUPER-e.

For the study of heavy, neutron-rich nuclei the main efforts this year have been in preliminary measurements with LINAC-accelerated beams intended to explore the optimum conditions for population of high-spin isomers using deep inelastic reactions. As well we used selected incomplete fusion reactions to study heavy nuclei such as ^{213}At and ^{211}Bi for which other spectroscopic information has been obtained from Gammasphere experiments with deep-inelastic reactions. One focus of these studies is the identification of configurations which involve the valence particles outside the N=126 and Z=82 cores. Results for the 2-proton hole case ^{206}Hg from the same study have now been published in Physical Review Letters, part of a continuing collaboration with the Cracow, Berkeley, Argonne groups and ourselves.

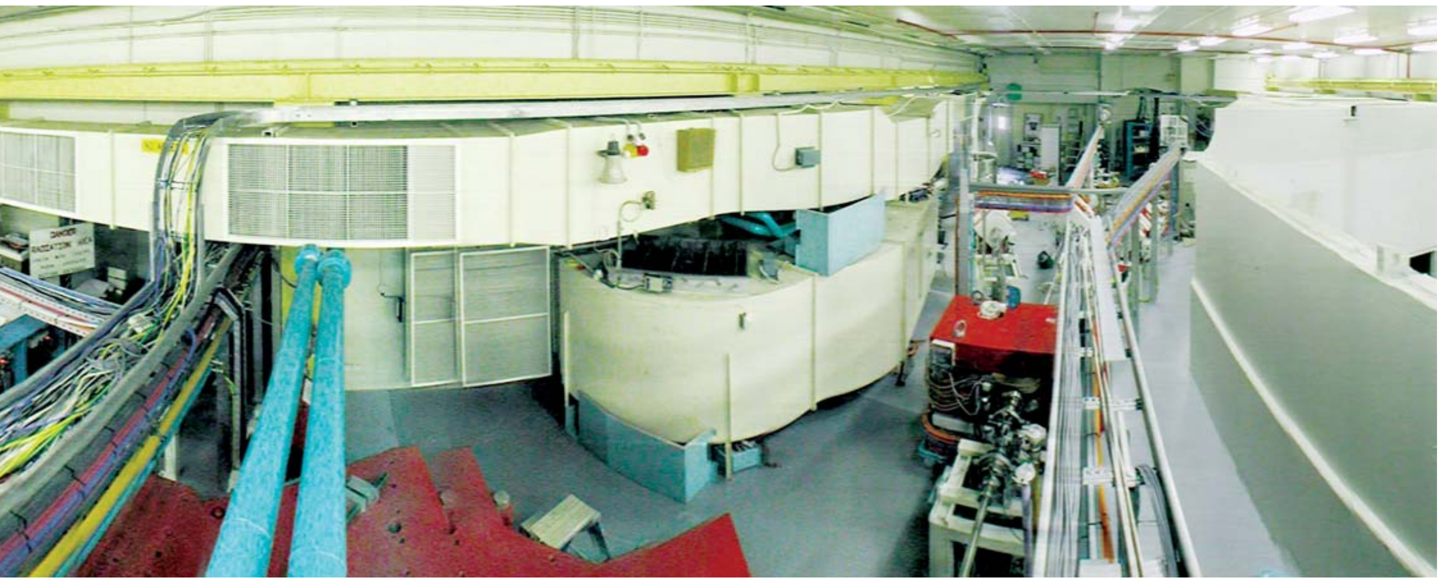
Details of these and other spectroscopic studies are available in the Department Annual Report.

In the area of instrumentation further developments of the electron-detector array, HONEY, to be used in the superconducting solenoid for broad-range electron-electron coincidences have been carried out. The γ-ray array CAESAR is being augmented with new detectors which are currently under test. Considerably improved efficiency should be available in early 2002. Parallel developments in the data acquisition system required to cope with the higher rates and to improve generally the flexibility for using ancillary detectors have been completed. (G.D. Dracoulis, A.P. Byrne, R.A. Bark, T. Kibédi, G.J. Lane, A.N. Wilson, J.C. Hazel and P.A. Davidson)

Magnetic Moments and In-Beam Hyperfine Interactions

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

A spectrometer for studying hyperfine interactions is being constructed by means of funding from a RIEF grant with collaborators from ADFA, The Faculties and Melbourne University. The cryocooler, most of the signal processing electronics and many of the data-acquisition components have been purchased. While the spectrometer is under construction, the research program is focusing on the measurement and interpretation of nuclear moments, and the development of BaF_2 detectors for fast-timing applications to nuclear spectroscopy and hyperfine interactions research.




Martin Robinson working in the target area

A new technique to measure the magnetic dipole moments and electric quadrupole of short-lived (sub-nanosecond) excited nuclear states in neutron-deficient nuclei has been developed over the past few years. It is based on the measurement of perturbed directional correlations of gamma-rays emitted from nuclei that have their spins aligned by a heavy-ion fusion-evaporation reaction. The angular correlation formalism developed for the analysis of the data has been accepted for publication and the analysis of the first set of measurements, on the neutron-deficient platinum isotopes ^{180}Pt, ^{182}Pt and ^{184}Pt, has been completed. The g factors of the lowest 2^+ and 4^+ states were measured, as were the average g factors of the high-spin quasicontinuum in each isotope. The observed quasicontinuum g factors in the platinum isotopes are almost a factor of two larger than those measured for other nuclei in the region, which indicates the importance of proton configurations at high spin in these nuclides. The fact that this inference is consistent with the discrete spectroscopy has alerted us to the possibility that strong correlations between the magnitude of the quasicontinuum g factor and features in the discrete spectroscopy may be a general phenomenon, which requires further evaluation and investigation.

A number of collaborative investigations are underway which focus on the measurement and interpretation of nuclear moments in semi-magic nuclei and their neighbours. For example, in collaboration with colleagues from Rutgers University, University of Bonn and Lawrence Berkeley National Laboratory, the magnetic moments of excited states in the xenon isotopes ^{130,132,134,136}Xe have been measured by the projectile-excitation transient-field technique. Pronounced variations in the excited-state g factors occur near the closed-neutron shell nucleus ^{136}Xe, but these variations disappear with the onset of collectivity as the number of neutron holes increases. Shell model studies have been performed to identify the main configurations that give rise to pronounced g factor variations near the closed shell and to explore the evolution of the collective structures.

Considerable effort has been invested this year in developing BaF_2 detectors for fast-timing experiments in-beam. The eventual aim is to exploit the pulsed beam from the Linac and use the excellent timing characteristics of BaF_2 detectors to measure high-frequency Larmor precessions for nuclear states implanted into ferromagnetic hosts. The initial developments in association with the nuclear spectroscopy program, have focused on nuclear lifetime measurements, which are conceptually simpler. Most of the technical problems have been solved and the first sub-nanosecond lifetime measurement by direct timing techniques in-beam gave a lifetime for the first-excited state in ^{184}Pt to a precision of better than 5%. (A.E. Stuchbery, A.P. Byrne, G.D. Dracoulis, R.A. Bark, A.N. Wilson, P.A. Davidson, A.M. Baxter, M.P. Robinson and D. Mitchell)

Perturbed Angular Correlations and Hyperfine Interactions in Materials

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

The study of semiconductor materials characterised with the Perturbed Angular Correlation (PAC) method has continued this year with measurements using both ^{111}In and ^{100}Pd radioactive probes. In both cases the radioisotope was introduced into the sample by a direct production/implantation technique using beams from the 14UD accelerator, followed by an annealing sequence to remove damage associated with the introduction of the radioisotope.

Gettering by layers of cavities in Si, produced by implantation of H or He followed by subsequent annealing, is a promising tool to prevent residual impurities, mainly transition metals, from degrading electron device performance. PAC studies of the morphology of the resultant cavities using the conventional ^{111}In probe are problematic due to the low mobility of the In atoms when implanted into Si. Work this year has focused on the development of alternative probes better suited to the study of cavities. One such probe is ^{100}Pd, whose physical properties more closely resemble the atoms normally gettered by cavities. The radioisotope has been produced using the ^{92}Zr(^{12}C,4n)^{100}Pd reaction. The probe has the disadvantage that the gamma-rays involved in the cascade lie close in energy and are not resolved by our detectors. Nevertheless, PAC spectra have been collected for a range of implants and work is underway to correlate the results with RBS measurements.

The investigation of diffuse disorder in semiconductors resulting from implantation using PAC has continued this year with measurements of the temperature dependence and background-dopant-concentration dependence of the hyperfine interaction in Si and Ge. At room temperature in undoped samples, the PAC spectra indicate that nearly all probes are on sites of nearly cubic symmetry. For samples with p-type dopant concentrations of 10^{18} and 10^{19} atoms cm^{-3}, the spectra show a perturbation associated with a broad range of frequencies. Previous studies of ^{111}In in Ge have associated such behaviour either with fluctuating electric field gradients or with the electronic state of the probe atom. Our results indicate greater attenuation is observed for the samples measured at liquid nitrogen temperature compared to those at room temperature. The general shape of the perturbation function is in good agreement with that predicted by a simple Monte Carlo model that places perturbing atoms diffusely on a lattice. (A.P. Byrne and N. Rao; M.C. Ridgway, D. Brett and A.S. Khalil [EME])

Accelerator Mass Spectrometry (AMS)

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

Demand for AMS measurements continues to be spread across a broad spectrum of isotopes including ^{10}Be, ^{14}C, ^{26}Al, ^{36}Cl, and isotopes of plutonium, with over 800 samples processed this year. It was a year of consolidation, with development effort going into refining the techniques for existing isotopes rather than developing new ones. In particular, measurements of all of the above isotopes now employ the gas stripper, with attendant improvements in transmission, consistency and ease of operation for those such as ^{36}Cl for which foil stripping was employed previously.

As in previous years, fields of application were diverse, and ranged across dating of early human occupation of the Indonesian archipelago, biomedical applications of ^{26}Al and plutonium, meteoritics, and tracing the vertical transport of plutonium in the oceans. Collaborative studies have involved a large number of users and contacts including a long-term postdoctoral visit funded under a Brazilian Government fellowship. Our vigorous collaboration with the Bureau of Rural Sciences has continued with measurements of ^{36}Cl in groundwater from wells in the Broken Hill and Temora areas. The latter is part of an exhaustive study of the groundwater issues, both physical and social, of this case-study area. In the course of a visit by scientists from Middlesex University and the University of Kazakhstan, a large number of samples from a long-term biomedical study of plutonium retention by humans were measured, as well as the first samples from a project studying the Semipalatinsk test site in Kazakhstan.

Considerable effort continues to go into ^{10}Be for a project on landscape denudation and sediment storage at a range of scales throughout the Australian continent, as well as extending the scope of the study of the glaciation history of Tasmania. This project is a collaboration with RSES, and a substantial data set has now been accumulated and is being interpreted. In addition, in collaboration with a group at Edinburgh University, ^{10}Be and ^{26}Al samples have been measured for studies of glacial advance and retreat and landscape evolution in Scotland and the western USA.

This year, radiocarbon projects constituted about 25% of the samples measured. New archaeological projects in Brazil, Sarawak and Flores were undertaken, and in collaboration with CSIRO Land and Water, groundwater ages were determined for several projects.

In addition to the work at the ANU, Dr Fifield spent 3 months at ETH, Zurich where he explored the potential of a small 0.5 MV AMS system with a view to expanding the AMS capability of the Department by the purchase of such a system. It would be very attractive for measuring some of the isotopes presently measured with the 14UD, in particular ^{14}C, ^{26}Al, ^{129}I and possibly plutonium, offering high precision together with simplicity of operation and a high level of automation. (L.K. Fifield, S.G. Tims, G.M. Dos Santos, T.T. Barrows and V. Levchenko)

Heavy Ion Elastic Recoil Detection Analysis (ERDA)

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

Research activities in this area this year included the compositional analysis of technologically interesting materials and thin films as well as fundamental experiments on detector response. A highlight of the year was the International Conference on Ion Beam Analysis in Cairns which was co-organised by the group.

Non-stoichiometric silica films have been analysed with respect to excess Si and H content. The excess Si, which can be well quantified with heavy ion ERDA, is related to the photoluminescence properties of the material.

Happy nuclear physicists - the staff and students of the Department

The collaboration with Macquarie University to investigate the deposition process of polycrystalline GaN films has been continued. A major outcome of this work has been that in these films O content and average crystal size are correlated. This indicates that the contaminant O is dominantly located at crystal boundaries. Polycrystalline GaN films are being developed as an alternative to expensive single crystalline material for applications in optoelectronics, such as blue LEDs.

The group participated in a Round Robin study of H depth-profiling using ion beam analysis techniques by contributing ERDA results obtained with an incident beam of 200 MeV Au ions. This international study, which included 8 laboratories, produced valuable insights about the relative advantages of the different ion-beam techniques with regard to H analysis.

Measurements of the pulse-height deficit effect in gas ionisation detectors have been continued using different gas pressures in order to establish if the effect depends on the density of the ionisation plasma. In addition, the effect of the deficit on depth profiling with elastic recoil detection has been investigated using well-defined triangular dopant profiles. It was found that for heavy ions and larger depths the uncertainty introduced by the deficit is significant and has to be considered in the depth calibration. (H. Timmers and T.D.M Weijers; R.G. Elliman [EME])

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Optical Sciences Centre

Professor Allan Snyder - Head of Optical Sciences

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

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

Research Summary

This was a special year with research continuing in new directions, and a number of significant achievements.

We have ventured into the new area of mind physics. The intent is to research universal aspects of brain processing. This is in conjunction with the new laboratory at the Centre for the Mind.

Professor Allan Snyder was jointly awarded the world's "foremost prize in communications and information technology", the Marconi International Prize, shared with Bell Laboratory's pioneering optical physicist, Dr Herwig Kogelnik. The award ceremony was in New York City on 4 December.

To celebrate the 100th anniversary of the first trans-Atlantic wireless transmission, Professor Snyder delivered the Royal Society's Clifford Paterson Prize Lecture. His lecture presented on 10 December in London, was entitled "Light guiding Light into the new Millennium".

Below we mention some of our recent activities and collaborations.

Research Accomplishments

Pulsating Solitons, Chaotic Solitons, Period Doubling, and Pulse Coexistence in Mode-locked Lasers: CGLE Approach

The complex Ginzburg-Landau equation (CGLE) is a standard model for pulse generation in mode-locked lasers with fast saturable absorbers. Complicated pulsating behaviour of solitons of the CGLE and regions of their existence in the 5-dimensional parameter space were found. Zero-velocity, moving and exploding pulsating localised structures, period doubling (PD) of pulsations and the sequence of PD-bifurcations were presented. Chaotic pulsating solitons were also found. Regions of parameters of the CGLE where pulsating solutions exist were plotted. The coexistence (bi- and multi-stability) of different types of pulsating solutions in certain regions of the parameter space of the CGLE was demonstrated. (N. Akhmediev and J.M. Soto-Crespo; G. Town [University of Sydney])

Observation of Soliton Explosions

We showed, experimentally and numerically, that Ti:sapphire mode-locked lasers can operate in a regime in which they produce exploding solitons. This happens when the laser operates near a critical point. Explosions occur intermittently. They happen spontaneously, but external perturbations can trigger them. In stable conditions of operation, all explosions have similar features, but are not identical. The characteristics of the explosions depend on the intracavity dispersion. (S.T. Cundiff [University of Colorado,USA]; J.M. Soto-Crespo and N. Akhmediev)

Soliton States in a Nonlinear Directional Coupler with Intermodal Dispersion

We studied numerically the propagation of short optical pulses in a nonlinear directional coupler that possesses significant intermodal dispersion. Using the split-step method with fast Fourier transform, we calculated the soliton solutions of such a coupler and highlighted the effect of intermodal dispersion on the propagation dynamics of the pulses. We found that the intermodal dispersion has only a small effect on the shape of the soliton states, in spite of the fact that it can distort and break up low-energy pulses launched into one arm of the coupler. The intermodal dispersion, however, can cause a drift in the velocity of the soliton pulses. (V. Rastogi and K.S. Chiang [City University of Hong Kong]; N. Akhmediev)

Professor Allan Snyder as a subject in his own experiments, using TMS in an attempt to boost dormant brain processes

Radiation-Related Polarisation Instability of Kerr Spatial Vector Solitons

We report the experimental observation and numerical simulations of a polarisation instability of spatial vector solitons in an AlGaAs slab waveguide. At power levels where the nonlinear index change becomes comparable to the birefringence, the fast soliton becomes unstable. The instability is related to coupling of the fast soliton to the slow radiation modes via phase matching. The combined effects of bifurcation and radiation coupling are the processes ultimately limiting the stability of any single-polarisation (fast and slow) Kerr soliton. (R.R. Malendevich, L. Friedrich and G. Stegeman [CREOL, USA]; J.M. Soto-Crespo and N. Akhmediev; J.S. Aitchison [University of Glasgow])

Simultaneous Existence of a Multiplicity of Stable and Unstable Solitons in Dissipative Systems

Dissipative systems are found to have multiplicity of stationary solutions in the form of both stable and unstable solitons. Most of the soliton solutions are unstable. However, all types of solitons play an important role in general dynamics of the system. We have also found that solitons can be unstable in parts. (J.M. Soto-Crespo and N. Akhmediev; K.S. Chiang [City University of Hong Kong])

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Plasma Research Laboratory

Professor Jeffrey Harris - Head of Plasma Research Laboratory

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

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

Research Summary

The Plasma Research Laboratory (PRL) as a department comprises two major activity areas, the Toroidal Plasma Group and the Space Plasma and Plasma Processing Group (SP^3). Its research also involves the Plasma Theory Group through collaborations with the Department of Theoretical Physics and the Faculty of Engineering and Information Technology. Professor Jeffrey Harris the Head of the Laboratory and the Toroidal Plasma Group, Professor Roderick Boswell is leads the SP3 Group, and Professor Robert Dewar leads the Plasma Theory Group.

The Laboratory conducts fundamental and applied research in the behaviour and use of ionised gases—plasmas—using its extensive facilities. These include the H-1NF heliac, a large toroidal confinement device, which became a Major National Research Facility in 1997, linear plasma machines based on the helicon plasma source concept developed by the Laboratory, high-power microwave and radio-frequency plasma heating systems, and extensive multi dimensional diagnostic and data acquisition systems. Its unique facilities and the wide ranging interests and collaborative connections of the research staff make the Laboratory a national resource and place it among the leading university-based plasma physics laboratories in the world.

PRL's research activities fall into four main areas:

Turbulence, stability, transport and flows are investigated using probe, spectroscopic, and microwave diagnostics. The main goal is to understand microscopic mechanisms of the interaction between the plasma free energy, turbulent fluctuations and the particle and energy transport, using the heliac plasma as an experimental target for diagnostics including electric and magnetic probes, multi-channel spectroscopy, collective microwave scattering diagnostic and others Among recent physics highlights are the discovery of the non-ambipolarity of the turbulent transport and detailed studies into the dynamics of the interaction between turbulence and electric fields in the plasma.

The interaction of plasmas with electromagnetic waves is studied in the context of plasma production and heating in both linear and toroidal magnetic fields and also for wave propagation and plasma diagnostics. These phenomena are also crucially important in a number of technological applications, including plasma sources for materials processing, plasma antennas, plasma thrusters, and wireless communications

Plasma diagnostics are essential for all these experiments, and the Laboratory is active in developing a number of different diagnostic techniques. These include novel probe techniques for studying turbulence, electric fields and potential structures, plasma flows, and species distribution functions; optical techniques such as tomographic and crossed-sightline spectroscopy and imaging Fourier transform spectroscopy; microwave techniques such as tomographic interferometry, scattering from turbulent density fluctuations, and reflectometry. These diagnostic instruments produce a huge variety of signals for which special acquisition and analysis methods are developed using digital signal processing techniques including cross-power spectral and wavelet analysis, virtual instruments, and data-mining.

Technological applications arise naturally from plasma physics research because of the multi-disciplinary nature of the field. Applications under investigation in the Laboratory include:

- the use of helicon plasma sources for thin-film processing for optical waveguides
- plasma antennas for communications and radar
- high-speed visual and infrared spectroscopic imaging for industrial applications
- plasma thrusters for space travel
- VHF wireless Internet communications for rural Australia
- 3-D visualisation of data, computer simulations and virtual reality

Research on these applications is supported by a variety of contracts with sponsors including the Australian Defence Science and Technology Organisation (DSTO), the Commonwealth Scientific and Industrial Research Organisation (CSIRO) and industrial partners in Australia and overseas.

Highlights of the individual research pursuits within these areas are described in the following sections. In all cases, research projects involve close teamwork of staff and students under the supervision of a senior research staff member.

Development of the H-1 National Facility

This year the heliac, the centrepiece of the H-1NF, was operated for 115 days over 40 weeks, recording 52 Gigabytes of data over 4,400 shots. Of this, approximately 3,700 shots over 97 days of operation were plasma physics shots, the balance being power supply and machine test shots. The high-precision 12 MW magnet dual power supply will ultimately increase the magnetic field of the H-1NF device from its original operating value of 0.2 T to its design value of 1 T. This year, a program of tests at 0.5 T, with very sensitive magnetic diagnostics, in combination with new power supply control software, has demonstrated control to a small fraction of 1 A, and extended the sensitivity of measurements to equivalent currents about one order lower. The high precision of the power supply ensures highly accurate magnetic geometry, avoids interference with measurement systems, and minimises induction of current into this inherently current-free plasma configuration.

The flexibility of the H-1NF is obtained though a secondary supply which powers the control windings and allows the plasma shape to be varied, under computer control, over a much wider range than possible in conventional stellarators or tokamaks. This year, by using the new power supplies, the flexibility of magnetic configurations was explored over a much wider range than ever before, in much more detail, and much more straightforwardly. Initial results show an optimum configuration for plasma density at about 20% higher vertical field than the original design, and some variation with the current in the helical core. The effect of magnetic configuration changes on magnetic fluctuations is being explored as part of the thesis work of PhD student David Pretty.

Regular plasma operation at 0.5 T (~1400 pulses) provided the highest densities in H and He so far obtained in the H-1NF – more than 10 times higher than before ($\langle n_e \rangle > 2\times10^{18}$). The best results were with RF heating near the ion cyclotron frequency (7 MHz) in H and a H-He mixture. As well as being of intrinsic interest, this provided a target plasma for the first phase of high temperature plasma operation in which the plasma is heated at the second harmonic of the electron cyclotron resonance frequency.

The 28 GHz, 200 kW electron cyclotron heating, recently recommissioned as part of the collaboration with Kyoto University and the Japanese National Institute for Fusion Science (NIFS), was tested to full power, and brought into regular operation onto a plasma target . After some initial problems with the high-voltage oil tank, the gyrotron was successfully operated very close to full ratings in power and pulse length into a test load. Reliable operation into plasma was achieved at about 100 kW power for 10 ms, or up to 20 ms at lower power. The clearest result is a rapid increase in plasma density. More success at increasing plasma temperature is expected once the gas input can be more accurately controlled and impurity levels are reduced. Initial impurity control is aimed at water vapour reduction by means of moderate (40-70ºC) baking of the coil set. A capacitor bank has been installed to increase the gyrotron pulse length to 40 ms.

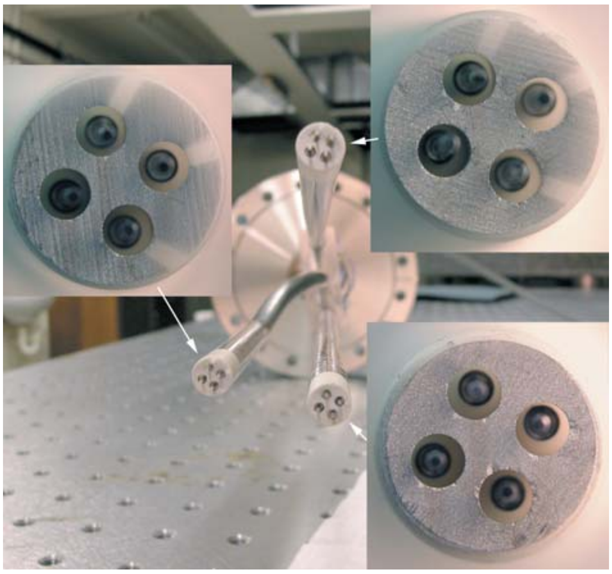
Work on the ion cyclotron range heating system included installation and characterisation of DC isolation components, and cabling with high-power coaxial cable to the launching port and optically-isolated pulse control electronics. A full remote control system will be installed next year.

To improve pumpdown after vacuum breaks, a cryopump was commissioned in early 2001, producing an order of magnitude improvement in vacuum quality in normal operation. This pump is designed to have a high capacity to pump water vapour, and uses a simple, large-area cooling coil instead of critical activated surfaces which can be easily contaminated. This, and similar redundancy or alternatives in the power and heating systems, has provided a very high level of availability this year, and will facilitate the remaining upgrades to the heating and launching systems. The final step, that is bringing the magnetic field up to

Panorama of H-1NF showing installed ECH microwave waveguide system full strength (1 T), is expected to consume less than three months of machine time, mainly for mechanical and electrical tests.

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

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



Multi channel plasma probe arrays used for turbulence studies in H1-NF

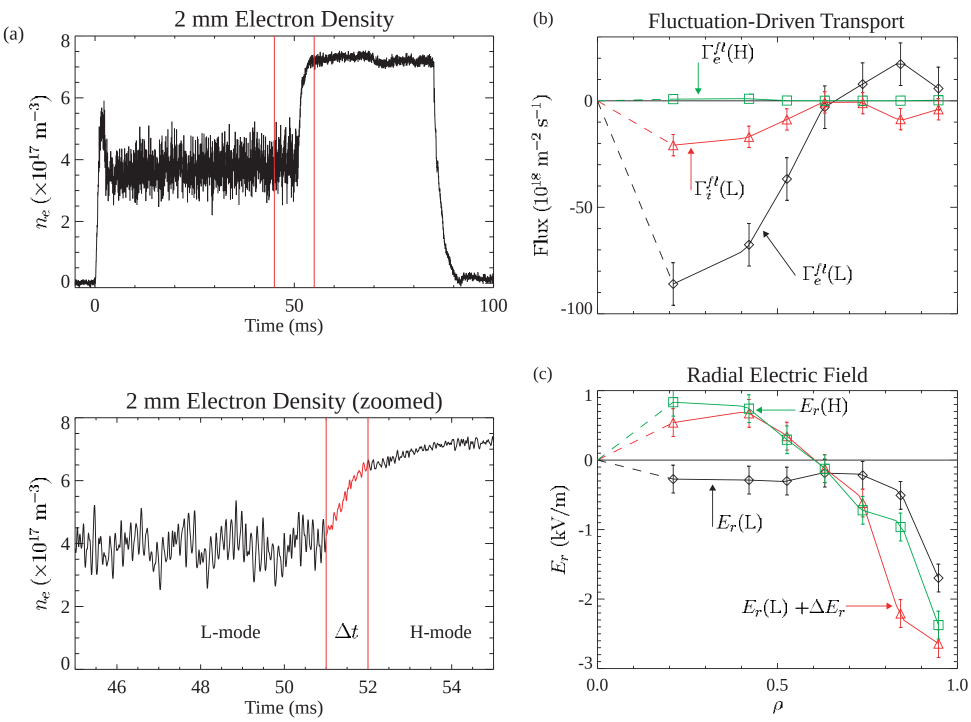
Toroidal Plasma Physics

Transport and Turbulence Studies in the H-1NF

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

Understanding a complex interplay between plasma fluctuations and flows is as interesting from the practical point of view (improved transport properties of magnetic confinement experiments) as it is for the fundamental plasma physics. Among the breakthroughs in 2001 is a new result on the nonambipolarity of the fluctuation-driven transport. It has been demonstrated experimentally that the turbulence can generate plasma flows. Plasma fluctuations transport electrons and ions across the confining magnetic field at different rates thus generating a radial electric current. This current changes the radial electric field in the plasma. When a sufficiently high gradient of the radial electric field builds up, the resulting shear flow suppresses the turbulence and brings the plasma to a higher confinement level as seen below This discovery changes our understanding of the turbulence-flow interaction, supporting to some extent the idea of turbulence self-regulation.

New multi-channel electric probe arrays shown in have been designed and fabricated to continue experimental studies into turbulence and transport in the H-1NF. A 20-channel visible spectroscopy diagnostic is also being successfully applied to



Radially resolved probe measurements during an H-1NF plasma shot in which an L-H confinement transition occurs: (a) discharge waveforms; (b) profiles of particle fluxes and (c) radial electric fields in H-1NF, showing reduction of outward turbulent particle flux at L-H transition and simultaneous changes in electric field driven by the turbulence.

studies of the effect of turbulence on the plasma profile evolution. (M.G. Shats, W. Solomon, H. Punzmann and H. Xia)

Transport Studies by Electrode Biasing

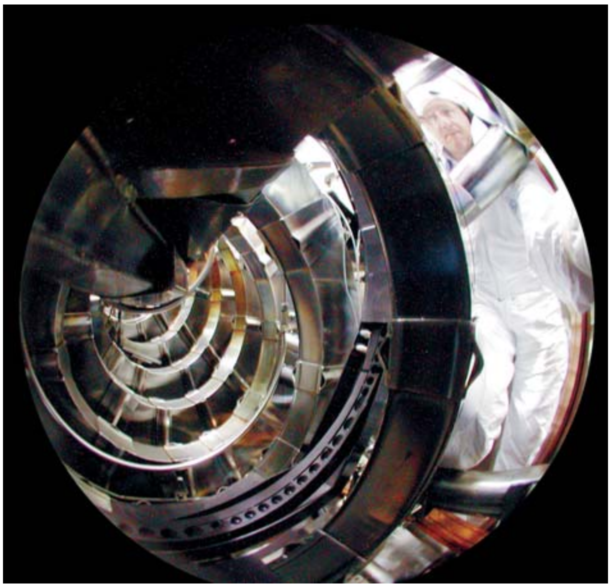
Plasmas over a range of magnetic fields have been electrically biased using an internal electrode to drive radial electric current. The initial goal of the experiment is to attempt to modify transport by changing the internal radial electric field. A number of measurement systems, including the tomographic interferometer, MOSS camera and various electrical probes have been used to study the plasma response. Modifications to plasma confinement are pronounced and the measurements indicate strong flow damping in the H-1NF that cannot be readily explained by neoclassical viscosity or collisional momentum dissipation. (B.D. Blackwell, J. Howard, H. Punzmann, I.H. Hutchinson, C. Michael and J.H. Harris)

Magnetic Design and Optimisation/Advanced Stellarators

As part of the collaboration on Stellarator Optimisation with Princeton Plasma Physics Laboratory, ANU has developed an optimisation procedure for auxiliary windings on stellarators. This is an extension of the BLINE code – an object-oriented vacuum magnetic-field line tracing code with real-time stereoscopic display of field lines and conductor elements. This program, when instructed to compute the optimum element for adjusting rotational transform, has “re-invented” the “flexible heliac” configuration originally discovered using manual methods by Harris et. al, and incorporated in the H-1NF design as the ‘helical coil’. New auxiliary windings are now being explored. This program has been added to the compact disk containing the H-1NF magnetic field data and the interactive tracing program in web browser format will prove useful to collaborators who need to understand the H-1NF magnetic geometry in detail. (B.D. Blackwell , B.F. McMillan and J.H.Harris)

Interferometry

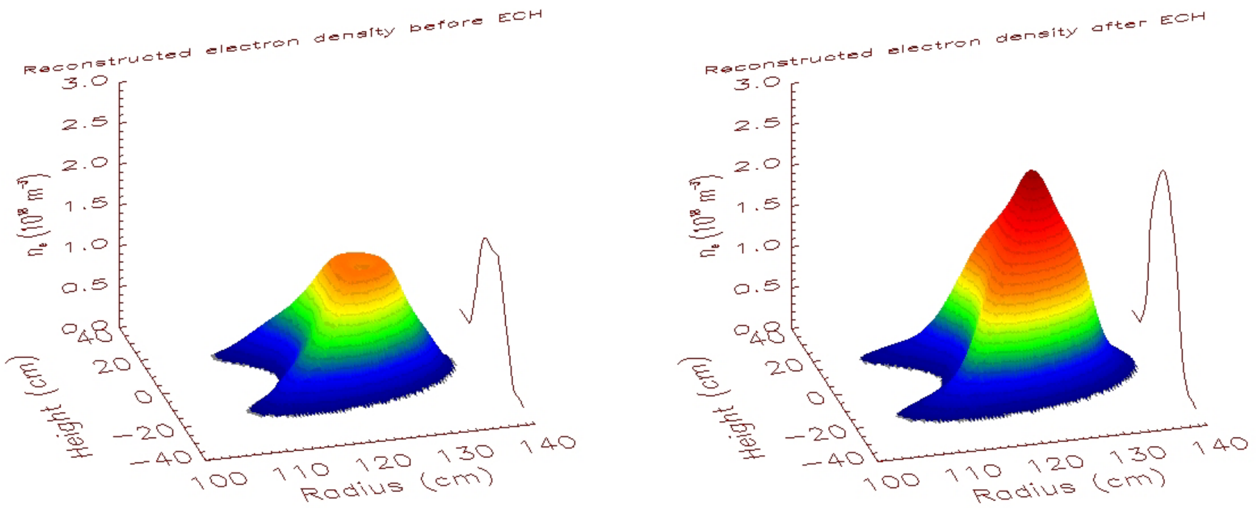
The far-infrared (FIR) and millimetre wave interferometers continue to operate reliably and have provided basic electron



A view down the coils of H1-NF towards the new 55-channel visible spectroscopy diagnostic (perforated black ring)

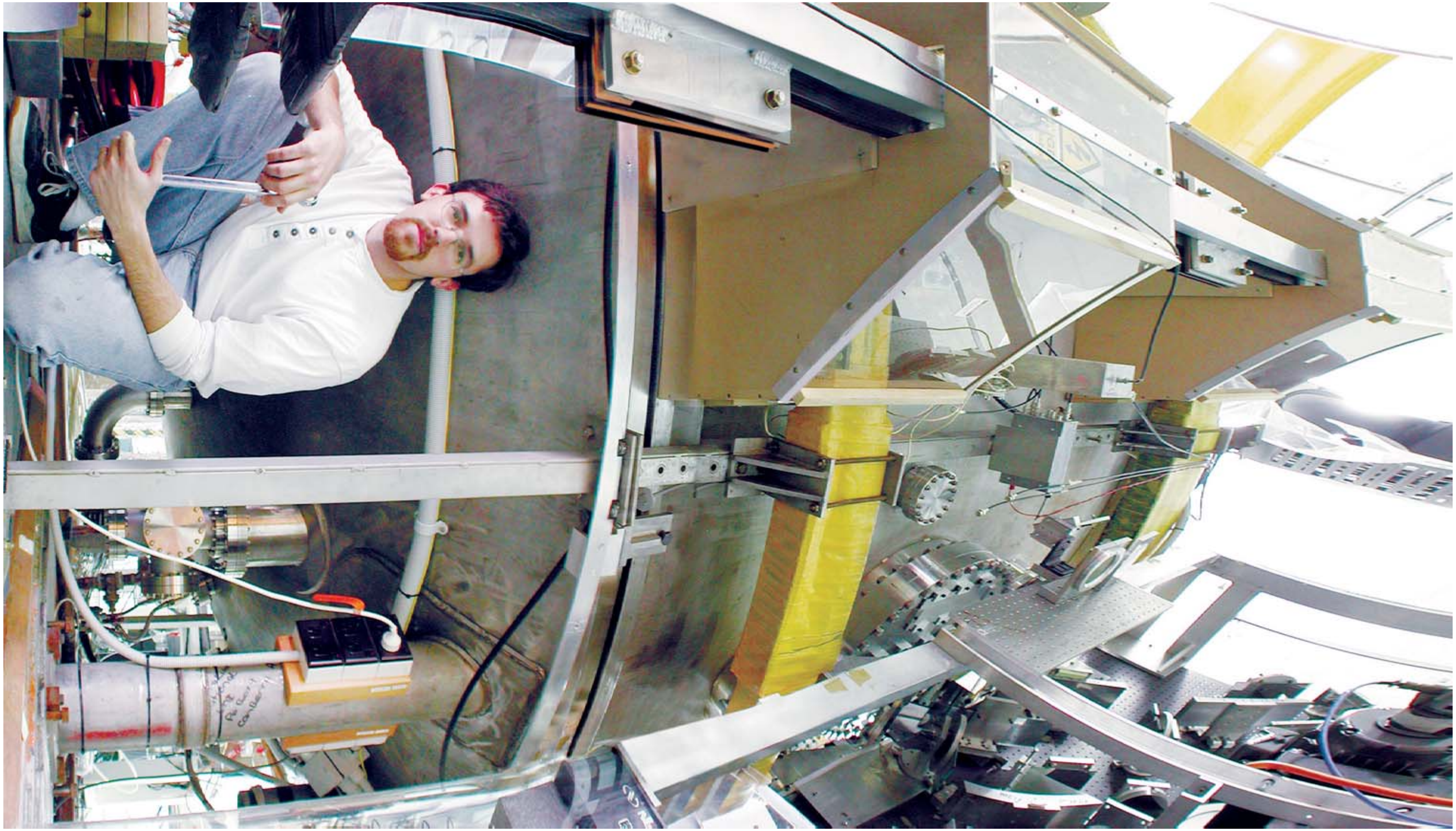
density profile information important for understanding the physical behaviour of the H-1NF plasmas. The 2 mm system provides a routine measurement of the line-integrated plasma density. Profile information is obtained using the 2D scanning FIR tomographic interferometer. The powerful imaging capability has been particularly useful for particle confinement studies in recent experiments involving the perturbation of the plasma by a moveable electrically-biased probe. Representative results are shown below.

An important step towards reliable tomographic analysis has been the development of suitable algorithms for relating laboratory space coordinates to plasma magnetic coordinates. A new database of computed vacuum magnetic configurations has been established that will allow reconstructed plasma density profiles to be available soon after the completion of each plasma discharge. (C. Michael, S. Collis and J. Howard)



Tomographically reconstructed density profiles of heliac plasmas before (a) and during (b) electron-cyclotron heating.

A worm's eye view of the H1-NF. Fenton Glass attends to maintenance of the multi channel optical tomography system



Spectroscopy

A number of advanced diagnostic measurement systems based on the MOSS spectrometer are now operating routinely. The MOSS, which has been patented by the ANU, is a modulated fixed-delay Fourier transform spectrometer based on solid electro-optic birefringent components. It is used for polarisation and Doppler spectroscopy of transition radiation from neutral atoms and from ions.

Recent highlights and developments are outlined below.

- The MOSS camera has been upgraded from 16 to 32 channels for high spatial/temporal resolution studies of ion and atom velocity distribution functions in the H-1NF. The high temporal resolution allows studies of ion dynamical behaviour on time scales comparable with the ion energy confinement time. Careful studies using a high-resolution grating-based McPherson spectrometer have confirmed ion-temperature results obtained using the MOSS camera, though without time resolution.

- The camera has been used to study hysteresis of the plasma dynamics under conditions of strong and weak dissipation. It has also been used for basic scaling studies of plasma ion temperature (versus magnetic-field strength, RF power and fill pressure), as well as providing essential information on the plasma flow dynamics during biased-probe experiments. Some representative data is shown on the right

- A new low-resolution, high-throughput grating spectrometer has been purchased as a flexible spectral prefilter for the MOSS camera. This allows significantly greater flexibility in the selection of radiating species for ion-temperature measurements.

- Work has continued with the tomographic MOSS system (ToMOSS), which is based on a rotatable platform that supports an array of 55 lens-coupled optical fibres that view the H-1NF plasma cross-section. The light signals are transported to a 2D MOSS camera for spectral processing.

- A benchtop system for Zeeman spectroscopy has been constructed and tested successfully. The instrument has application for sensitive and fast measurement of current profile in large tokamaks (e.g. DIII-D) as well as in solar astrophysics. This work was a central component of a Masters thesis "Measuring magnetic fields using light" by A. Danielsson from Chalmers University in Sweden.

- A high-resolution survey spectrometer has been commissioned for study of plasma impurities, species ionisation states and spectral lineshapes. The system has been recently calibrated against an atlas of known emission lines from many atomic species. The data provide a useful comparison for MOSS and camera systems.

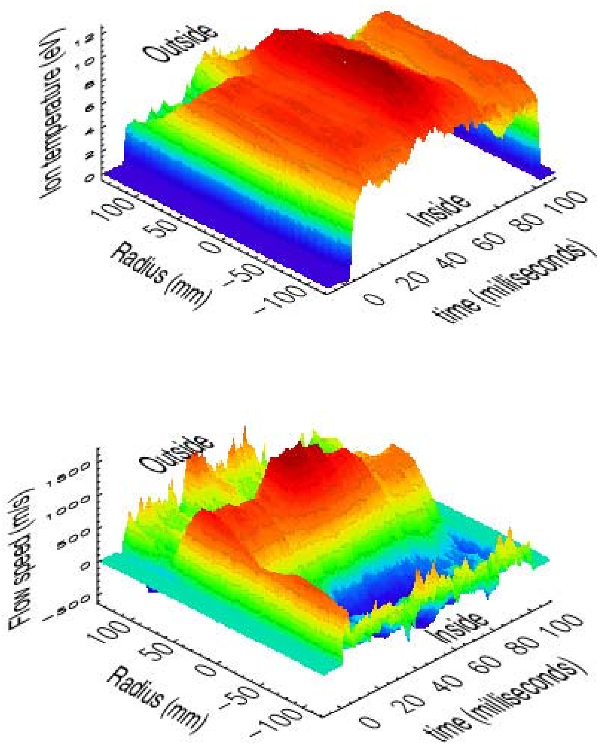
This year has also seen the development of high-throughput, visible-near-infrared modulated interferometric sensors for remote temperature measurement. The new electro-optic filters offer an attractive alternative to traditional radiometric systems and are the subject of provisional patent protection. PRL has negotiated a contract with DSTO for the development of imaging interferometric sensors for the infrared discrimination of rocket and engine infrared signatures. (J. Howard , C. Michael, F. Glass, B. Blackwell and R. Smeets)

Plasma Theory

Waves and Instabilities

The study of the spectrum of waves propagating or growing exponentially in the 3D geometry of the H-1NF is of great importance in understanding the behaviour of the machine, and is also of great theoretical interest because of the strong departure from symmetry in this machine. The fundamental issue is the fact that ray tracing in this and similar stellarators shows chaotic behaviour, in contrast to the regular behaviour found in tokamaks. Because of the analogy between plasma waves and Schrödinger waves, this is known as quantum chaos and how to handle this is still an open question in plasma physics. This is one way the national facility provides a stimulus for the theoretical plasma community in Australia.

One approach to calculating the spectrum is to expand the linearised perturbations of the plasma about equilibrium in a (truncated) complete basis set, leading to a large matrix whose eigenvalue spectrum is calculated numerically. This Galerkin approach is being pursued in a fully 3D resistive magnetohydrodynamic (MHD) model through the construction of the SPECTOR-3D code, which has been written and is being validated by comparison with simple cases previously studied. (R.G. Storer [Flinders University]; B. McMillan, H.J. Gardner and R.L. Dewar)



MOSS camera measurements of the plasma ion temperature (top) and flow speed (bottom) during heating power modulation experiments in argon at low field. The plasma makes a transition to higher confinement during the linear ramp-up phase 30ms into the discharge. The measurements have revealed a complex hysteretic behaviour as the input heating power is slowly ramped down from its peak value.

Ray Kimlin finally solves the instability problem on his instrumentation amplifier - it's just a matter of a big enough capacitor.

The principle test for quantum chaos is to show classical chaos in the semiclassical limit. By following the ray paths of short-wavelength ideal MHD waves calculated for the H-1NF, confined in a phase-space box that models the effect of numerical truncation of short wavelengths, it was shown that the problem is analogous to the quantum billiard problem and is similarly strongly chaotic. This means that there are no good quantum numbers – there is no simple pattern to the spectrum. However the tools of quantum chaos allow statistical predictions about the spectrum. By predicting the dependence of the instability spectrum on the short-wavelength cut-off, it is hoped that the theory will give a guide to the stability calculations in design studies for new machines, like the proposed Princeton NCSX device, and will also help estimate the region of physical applicability of MHD theory in existing experiments like the H-1NF. (R.L. Dewar, P. Cuthbert and R. Ball; M. Redi [Princeton University])

Before studying stability one must first have an equilibrium about which to linearise. In 3D geometries this is far from a trivial problem, even conceptually, due to the generically non-integrable nature of the magnetic field line system and the problem of distinguishing externally generated structure from that arising spontaneously from saturated instabilities. This is being addressed by calculating magnetic islands for both resistive-interchange-stable and -unstable H-1NF configurations with the HINT code, using the vertical field current as an external control parameter and the average plasma pressure as an internal control parameter. Evidence for incomplete self-healing has been found in the interchange-unstable case. (S.S. Lloyd and H.J. Gardner; T. Hayashi [National Institute for Fusion Science, Japan])

Confinement Transitions

The low-to-high (L-H) confinement transitions found experimentally on the H-1NF and many other toroidally-confined plasma devices also provide a stimulus for fundamental studies in the nonlinear dynamics of systems of coupled ordinary differential equations for the time evolution of variables describing the macroscopic state of the system (low-dimensional dynamical systems).

A mathematically and physically sound dynamical model that emulates many of the typical attributes L-H transitions in fusion plasmas has been elicited from an earlier flawed model, by considering the relationship between bifurcation structure, symmetry, and the physics of the process. The model contains two codimension-2 organising centres and two Hopf bifurcations, which underlie dynamical behaviour that has been observed but not mirrored in previous models. (R. Ball and R.L. Dewar)

Analytic and computational studies of this model have evinced two types of discontinuous transition that are qualitatively distinct. One is a hysteretic transition that may be quiescent or oscillatory. The other occurs as the consequence of a transcritical bifurcation when there is a significant shear flow drive. It is intrinsically oscillatory and non-hysteretic, and thus provides a model for the so-called dithering transitions that are frequently observed in magnetised plasmas. (R. Ball and R.L. Dewar; H. Sugama [National Institute for Fusion Science, Japan])

Novel Wireless Communication Technology

The Plasma Antenna

A DETYA Year 2000 Strategic Partnerships with Industry - Research and Training Scheme (SPIRT) grant was won by the Plasma Research Laboratory for further development of the HF plasma antenna in collaboration with CEA Technologies ACT (CEA) and NEOLITE NEON Sydney. The SPIRT grant is funding a PhD scholarship awarded to Liviu Lungu to undertake research in this area.

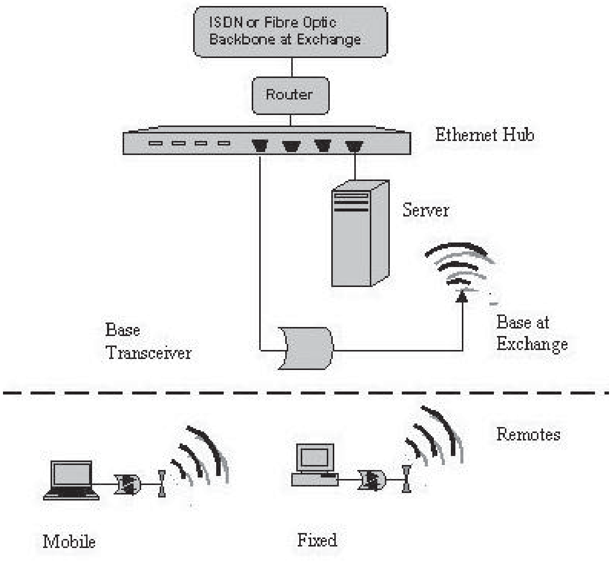
Collaborative work with CEA Technologies is being undertaken to develop techniques for energising plasma antennas without the need for RF drive. CEA wish to investigate the use of plasma antennas as highly adaptable antenna elements in arrays. Issues that need to be dealt with include noise power emitted by the power supply driving the plasma, the corruption of received signals by the noise generated by the plasma and the power consumed in forming the plasma.

The fundamental physics of plasma antennas is also under investigation. Work is continuing to endeavour to understand the low noise of RF produced plasmas and the origin of noise in DC discharges.

MOTOROLA Inc., USA has awarded the Plasma Research Laboratory a continuing contract of $49,500 to develop fast sub-miniature plasma switches for mobile phones. This grant is funding a PhD scholarship awarded to Peter Linardakis, who is investigating the RF properties of a simple plasma-based switch. He is performing a comparative investigation of plasma-based switches with the conventional technologies of PIN diodes and MEMS (micro-electromechanical systems) switches.

Wireless Communications

Eight fourth-year engineering students are involved in the development of a VHF wireless network for long-distance, high-data-rate communications. This work is motivated by the need to bring inexpensive, moderate-speed Internet service to regional Australia and is aimed at developing a system which exploits the Band I analog TV bands which are to be decommissioned at the end of simulcast in regional Australia



Schematic of proposed BushLAN VHF data communications system.

In the year under review, two projects have been completed: one on channel sounding studies based on a sliding correlator. This device allows the measurement of the maximum data rate that can be transmitted by the channel where multipath effects are the dominant limitation. A second project which saw the development of a DSP and a direct digital synthesizer (DDS) for data transmission has seen the investigation of the production of spread spectrum signals directly in software. This allows considerable simplification and versatility in the design of wireless transceivers. Work continued in 2001 on the complete implementation of a wireless network suitable for the provision of the Internet to regional Australia. The figure above shows a schematic for this concept which is called BushLAN (Bush Local Area Network). In the first instance, a simple network will be developed for deployment at VHF RSPhysSE to simulate the effects of Internet traffic between multiple users.

In 2001, PRL won $225,000 toward the purchase of state-of-the-art digital equipment for the study of digital wireless communications. These funds have been employed to purchase an AT89441A Vector Signal Analyser and ATE4433B digital RF generator.

Australian Fusion Research Group (AFRG) Collaborations

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

Plasma Theory

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

Soft X-Ray Measurement System

Final testing of the 16 channel soft X-ray system installed last year is nearing completion, preparatory to being set up as a permanent multi-channel diagnostic to monitor X-ray emission from 0.5 T ECH and RF produced plasma. A measurable high-energy X-ray flux is produced even with modest RF powers at 0.5 T in H plasma. (B.D. Blackwell and J. Howard; A.D. Cheetham, [University of Canberra])

High-Voltage Modulator for the MOSS Camera

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

Laser-Induced Fluorescence

This project received ARC funding for three years commencing in 2000. The aim of the project is to develop techniques for

The new HARE clean tent installed this year measuring electric fields in plasmas using the laser excitation and fluorescence of metastable He atoms in a pulsed He beam. Work undertaken by the Sydney group with collaborators at Hiroshima University (Professors K. Takiyama and T. Oda), has focussed on the development of a suitable metastable He beam injector. Measurements on the test source will be made later in 2001, while a collision rate equation model for He is being used to model the experiment. (B.W. James, P. Feng and D. Andruczyk [University of Sydney]; J. Howard)

Fibre Sensors

The University of New England developed novel optical fibre sensors and bolometers for electric field and thermal measurements in the edge and body of the H-1NF plasma. Their insulating nature and immunity to high voltage and electromagnetic noise makes these devices particularly attractive for plasma work. This collaboration was brought to a satisfactory conclusion this year with the PhD thesis submission by V. Everett. (V. Everett and G.A. Woolsey [University of New England]; J. Howard, B.D. Blackwell and J.H. Harris)

Space Plasma and Plasma Processing Group

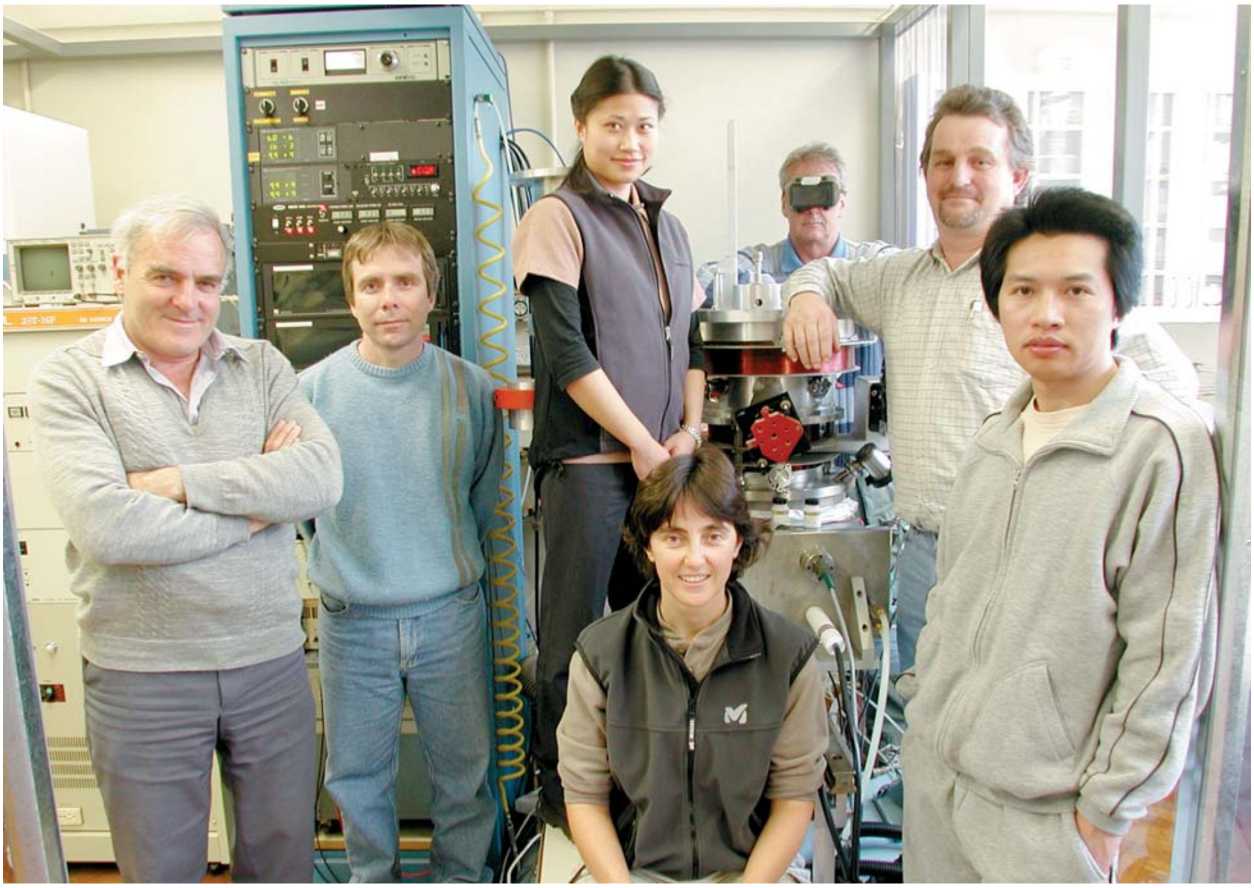
The SP^3 Group is primarily concerned with the basic physics of gaseous discharges and their application in the processing of thin films. Plasma modification of surfaces is one of the fastest growing areas of scientific research and industrial development in the world.

Basic Helicon Plasma Physics

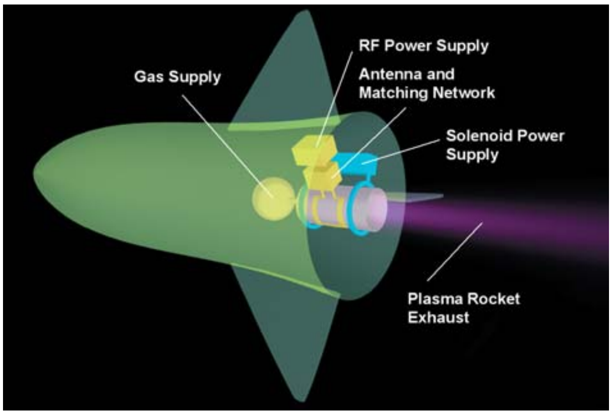
The interaction of plasma electrons with the helicon wave in the large plasma system 'WOMBAT' is being studied by correlating the spatio-temporal variations of bursts of AII emission with the wave fields in the plasma. The AII line has a lifetime about ten times shorter than the RF period allowing good phase measurements to be made. Under conditions where the helicon wave is propagating with a wavelength about equal to the source diameter bursts of AII emission travel down the source with the helicon wave strongly implying the wave fields are accelerating the electrons by a non-linear trapping interaction. Research has also shown instabilities associated with gas pumping and ionisation which leads to a transition from the inductive to helicon excitation. (A. Degeling, G.G. Borg and J. Scharer)

Optical Waveguides

In collaboration with Professor John Love from the Director's Unit, 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 Assisted Reactive Evaporation (HARE) for doping of silica films with Ge, for applications in active and nonlinear devices. The Group has reported the first UV-induced refractive index change in germano-silicate glass containing no detectable level of H. 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 effects. The primary thrust



Members of the HARE team



The high density helicon source which has possible applications in space propulsion

of the program has received a major boost with funding from the Photonics CRC to support three researchers, at present, and allowing us sufficient funds to renovate the laboratories. For the next couple of years the main aim is to produce waveguides for the 1.4 mm band, meaning the silica core must be completely water free. (C. Charles, Wei Tang Li, D. Bulla and R.W. Boswell; J.D. Love [DU])

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 three-crucible electron beam system from JEOL allowing the independent evaporation of Si and two dopants. Present research is focussing on the H free films and the machine conditions that allow its growth. A major problem was discovered with dust contamination which was improved by strict wafer handling and by the installation of a 'clean tent'. Considerable activity is now devoted to obtaining good quality dust-free material. (C. Charles, D. Bulla and Wei Tang Li)

Plasma Antenna Coupling

The helicon system "Chi Kung" is a research reactor for basic RF plasma phenomena. One of the problems of coupling RF power to a plasma is whether the antenna is isolated from, or in contact with, the plasma. The source end plate has been modified to allow a bare Cu antenna to contact the plasma. The original

Students explore the possibilities of the Wedge virtual reality theatre aim was to simulate the RF antenna in the H1-NF which is also in contact with the plasma and has a major effect on the plasma properties, but the system is also very similar to that used in industrial planning processing devices. Experiments to date have shown that the phase difference between the RF driving the helicon plasma generation antenna and the small antenna in contact with the plasma has a considerable effect on the plasma density and perhaps on the electron temperature. (A. Aanesland, C. Charles and R.W. Boswell)

High-Brightness Ion Source

We are working with a company in Boston, USA, to develop a high-brightness ion source using a helicon-excited plasma. The first milestone has been achieved experimentally. Our intention is to use this experience in ion sources to contribute to developing thrusters for space travel, and related modelling work is being carried out with colleagues in the USA and France. (O. Sutherland and R.W. Boswell)

3D and Stereo Data Visualisation Systems

Data visualisation plays an increasingly important role in interpreting scientific experiments and computer simulations. A considerable proportion of a research degree involves developing techniques to manipulate and view large sets of multi-dimensional data, and often this is difficult within the confines of a 2D screen. A two-screen rear–projection, immersive virtual reality theatre, the WEDGE, has been developed, and proved immensely popular. At present, a new WEDGE is operating in the Computer Science department of FEIT, a portable WEDGE is available and has been demonstrated in Melbourne, Wagga Wagga, Magnetic Island and Townsville. WEDGEs have also been installed in the Powerhouse Museum in Sydney, the Discovery Centre of the CSIRO in Canberra and the Australian Defence Force Academy. A new operating system based on Java 3D has been developed which we hope will be the basis of a linked WEDGE network.

A collaboration with the Centre for Visual Science has begun with a Masters student studying the effect of depth perception and steriopsis using a new WEDGE being developed out of the Robot Command Station. Using a digital light projector (DLP), polarisers and passive glasses, a simple table-top WEDGE can be constructed.

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John Howard, BSc PhD Syd

Fellows
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Gerard Borg, BSc PhD Syd
Henry Gardner, BSc Dip Comp Sci Melb, PhD (jointly with TP & Computer Science, FEIT)
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Technical Officer
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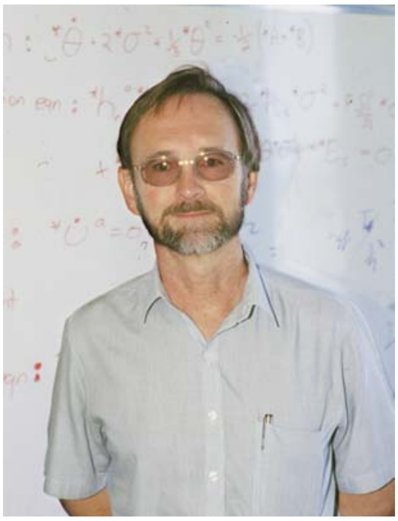
Theoretical Physics



Professor Robert Dewar
- Head of 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 Complex Systems it fosters multi-disciplinary research by organising topical research workshops, and plays an important national role in postgraduate education by holding annual graduate-level Physics Summer Schools.

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

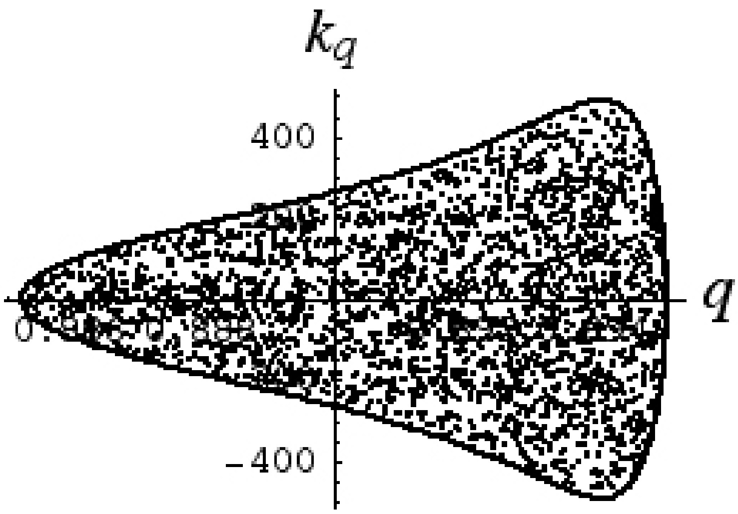
Research Summary

The Review of Theoretical Physics conducted in 2000 recommended a concentration of stand-alone research activity in the Department in the areas of condensed matter physics, mathematical physics and plasma physics, and the continuation of atomic and nuclear physics through joint appointment arrangements and Visiting Fellowships. A development not foreseen in the Review has been the move of the Protein Dynamics group from the Chemistry Department in the Faculties to the Le Couteur Building, thus greatly expanding the biophysics activity already underway in the Department. The format adopted for the Annual Report this year reflects the move towards greater focus into these six main areas.

Another development in 2000 has been the phased entry of the Institute of Advanced Studies into the National Competitive Grants program of the Australian Research Council. The Department has been very successful in this first round, with Professors Vladimir Bazhanov and Rodney Baxter receiving a grant of $318,000 over three years to investigate "Solvable Models on Regular and Random Lattices in Statistical Mechanics and Field Theory" and Dr S.H. Chung receiving $231,000 for "Theoretical Studies on the KcsA Potassium Channel and the L-type Calcium Channel". Professors Baxter and Bazhanov were also Chief Investigators in a grant of $457,836 administered by the University of Queensland to investigate "Algebraic Structures in Mathematical Physics and their Applications".

The Review also recommended the formation of a Division of Theoretical Physics (or Theory Division) to unify theoretical work in the School. Rather than create a new administrative layer, the School has decided to enhance the role of the existing Centre for Theoretical Physics as a unifying force within the School. As a signal of its broadened scope, and recognising the modern trend towards the study of emergent behaviour, the Centre has been renamed the Centre for Complex Systems, with the subtitle: Theoretical Studies: From the Cosmos to Quantum Systems, from Statistical Mechanics to Biophysics.

The Centre is supported administratively by the Department of Theoretical Physics and the academic staff of the Department play a major role in its activities. Centre activities this year were the 14th Canberra International Summer School on Biophysics: From Proteins to Cells, a Mini Summer School on Plasma and Gaseous Electronics, and the 25th International Workshop on Condensed Matter Theories, all convened by members of the Department with strong involvement of members of other departments.



Ray paths of the most unstable ballooning modes in the non-axisymmetric toroidal magnetic field of the H-1NF Heliac are chaotic as shown by the fact that intersections with a Poincaré surface of section fill the region ergodically.

Statistical Mechanics and Field Theory

Professor Rodney Baxter continued his study of solvable models in statistical mechanics and related areas of mathematical physics, finding a new invariant in the star-triangle form of the Yang-Baxter relation. There have been many papers written in the last thirty years which reveal basic misunderstandings of the Bethe ansatz. Professor Baxter has attempted to clarify these in a recent paper. (R.J. Baxter)

The continuous version of Baxter's commuting transfer matrix method has been developed for conformal field theories with the extended W3 symmetry. The results were applied to exact calculation of non-equilibrium transport properties for the quantum Brownian motion on the triangular lattice. An interesting connection of the results to the spectral theory of third-order differential equations has also been established. (V.V. Bazhanov and A.N. Hibberd).

Plasma and Nonlinear Physics

An integral part of designing a fusion experiment is to make sure that the plasma is stable, i.e., that small fluctuations are not amplified until they become so large they disrupt the plasma confinement. One theoretical approach to this problem is to calculate the frequency spectrum of the normal modes of oscillation (and possibly exponential growth) of the plasma. From a theoretical viewpoint, the study of the spectrum of small-amplitude waves in a stellarator (e.g. the Plasma Research Laboratory's heliac, H-1NF) is not very different from the study of the energy levels of Schrödinger waves in a molecule or non-circular quantum dot – they are all complicated "fitting waves in a box" problems. Thus the theory of "quantum chaos" may provide the basis for better understanding the difficulties encountered in the purely classical, but computationally challenging, numerical calculations of plasma stability. Further details of this work can be found in the Plasma Research Laboratory section on page 56 (S.S. Lloyd and H.J. Gardner; T. Hayashi [National Institute for Fusion Science, Japan])

Nonlinear Dynamics

A mathematically and physically sound dynamical model that emulates many of the typical attributes of low- to high-confinement mode (L-H) transitions in fusion plasmas has been elicited from an earlier flawed model, by considering the relationship between bifurcation structure, symmetry, and the physics of the process. The model contains two codimension-2 organising centres and two Hopf bifurcations, which underlie dynamical behaviour that has been observed but not mirrored in previous models. (R. Ball and R.L. Dewar)

Analytic and computational studies of this model have evinced two types of discontinuous transition that are qualitatively distinct. One is a hysteretic transition that may be quiescent or oscillatory. The other occurs as the consequence of a transcritical bifurcation when there is a significant shear flow drive. It is intrinsically oscillatory and non-hysteretic, and thus provides a model for the so-called dithering transitions that are frequently observed in magnetised plasmas. (R. Ball and R.L. Dewar; H. Sugama [National Institute for Fusion Science, Japan])

Bifurcation surfaces can illuminate dramatically the truism that what you see depends on where you view the object from. In this work, computed 3D surfaces of critical points are visualised for bifurcation problems that contain a pitchfork as an organising centre. It is shown by comparison of notionally equivalent problems how the ranges of discontinuous behaviour in nonlinear dynamical models (and the physical systems they purport to represent) are determined by other singularities that shape this surface. (R. Ball)

The mathematical methods of nonlinear dynamics can be applied in fields as diverse as plasma physics and chemical physics. As an example of the latter, the dynamics of micelle formation from amphiphilic monomers in non-equilibrium conditions may be emulated by an autocatalytic model, from which a coupled dynamical system is derived that incorporates non-trivial stationary states, multiplicity, and hysteresis. A singularity and stability analysis of this system showed how the hysteresis loop in non-equilibrium self-assembling systems could be used as an effective switch. This suggests new mechanisms for chemical information transfer, and potential applications in areas such as the design of tunable drug delivery systems, control of anaesthetic action, and operation of molecular switches in bioimmunoassay systems. (R. Ball; A.J.D. Haymet [University of Houston, USA])

Professor Coppel has completed the book on which he has been engaged for nearly six years, *Number Theory: An Introduction to Mathematics.* It consists of two volumes, each of almost 350 pages. It has been recommended for publication by the American Mathematical Society. (A. Coppel)

Biophysics

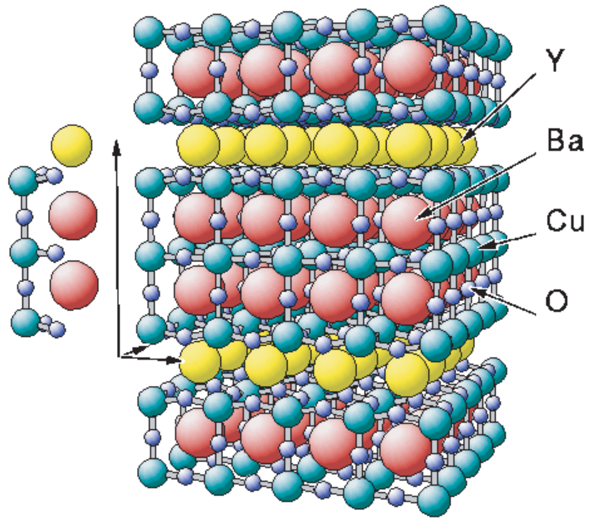
The properties of a potassium model channel that includes the full experimentally-determined protein with that of a simplified model are compared using Brownian dynamics simulations. In the simplified model, the irregular protein-water boundary was smoothed out and all the atoms forming the channel protein were represented as a homogeneous, rigid, low dielectric medium. It was demonstrated that the properties of the two model channels, deduced from electrostatic calculations and Brownian dynamics simulations, are qualitatively similar. Besides making the simulations easier, the study also helps in identifying the residues in the channel protein that have important effects in the permeation process. Mutations of such residues are expected to alter the conductance properties of the channel drastically, which can be easily measured in experiments. (S.H. Chung, T.W. Allen, S. Kuyucak and M. Hoyles)

An extensive series of studies was carried out on the gramicidin A (GA) channel, an antibiotic polypeptide that consists of 15 amino acids residues. Its structure has been known since the 1970s – it forms a 2 Å radius channel that extends for 25 Å, almost spanning the entire length of a membrane. While GA is not a biological channel, in the absence of other channel structures, it had become a de facto channel model in theoretical studies. Although numerous papers have been written on it in the past using various approaches, there are no systematic comparisons with experimental data that can be used to judge whether they are successful or not. A recent high-resolution atomic structure of the GA peptide was used in continuum electrostatic calculations, the observed properties of the GA channel could not be explained. The potential profiles for monovalent cations are found to be almost flat with no discernible wells at the pore entrances in contrast to the observed binding sites, and no central barrier that is essential in reproducing the saturation property. For divalent cations, the potential profiles consisted of only large barriers, which conflicts again with the observed binding sites at the pore mouth. Since the Poisson-Nernst-Planck equations and Brownian dynamics rely on continuum electrostatics to predict the channel properties from its structure, they cannot be used in modelling of the GA channel. This leaves molecular dynamics (MD) as the only alternative for this purpose. There have been dozens of MD studies of the GA channel to date, however, they all predict very large free-energy barriers for ions crossing the channel, which would make their conduction rate orders of magnitude smaller than the observe rate. A similar calculation of the potential of mean force for potassium ions using the high-resolution structure showed that an ion moving across the pore faces a 20 kT barrier. The problem in this case appears to be the neglect of polarisation effects in the MD force fields. Unlike bulk simulations of proteins, these are very important in ion channels because ions move from bulk to a narrow pore surrounded by protein, which has a very different polarisation characteristics than the bulk water. Thus a conclusion is that, at present, there are no valid theoretical framework within which one can attempt to study the GA channel. This calls for improvement of the MD force fields by including the polarisation effects. In the mean time, one could carry out an inverse study by constructing a potential profile that reproduces the known properties of the GA channel. This potential has an 8 kT well at the pore mouth but only a 5 kT central barrier (with respect to the well), much smaller than the predictions of the MD calculations. This potential profile will provide a useful guide in construction of polarisable force fields in future studies. The importance of such an effort, of course, goes beyond the GA channel as all channels have narrow pores and suffer from the same shortcomings in the MD force fields. (S. Scott, B. Corry, S. Kuyucak and S.H. Chung)

Condensed Matter Physics

Density Functional Theory of Super-Phenomena

Density functional theory is considered a standard model for low energy physics. The theory has a rigorous formal structure with a well-defined energy functional. In the past three decades it has delivered very impressive successes in the study of normal states of matter. However, 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 super-phenomena (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. At the Hartree mean-field level this theory has produced the well known BCS results. At present we are examining the adiabatic connection formula, which may be violated in presence of a phase transition. (M.P. Das)



$YBa_2Cu_3O_7$(.3) lattice

Electron Correlations

An investigation has been made on isothermal compressibility and long-wavelength static density-density response function of a weakly correlated 2D electron gas in the weak degeneracy regime. Here the Fermi temperature and the physical temperature are comparable. Preliminary results indicate that at a low density of electrons the correlation energy dominates over the exchange contribution. A further plan is to study the metal-insulator transition in 2D electronic systems by examining the behaviour of compressibility as a function of carrier density.

The problem of dynamical response and plasmon dispersion by adopting a nonlinear response function approach in a self-consistent manner has been studied. The main ingredient in the construction is the quadratic fluctuation dissipation theorem. The usefulness of this theory has been shown by using two simplifications, namely velocity average and dynamical superposition approximations. The reliability of the theory is assessed by observing that the principal coupling correction to the 2D temperature dependent Lindhard function is identified as being precisely the part of the third-frequency moment sum-rule coefficient proportional to the potential energy. (M.P. Das, K.I. Golden and F. Green)

Realistic models of many-electron correlations in 3D solids can now be solved using efficient algorithms and high-performance computers. An accurate evaluation of the self-energy operator with the screening of the interelectron interaction and vertex corrections can now be done on the basis of linear muffin-tin orbitals. This computational scheme proved to be very successful in describing the spectral function of various crystals composed of light s and p-electron atoms. Now this method is extended to heavier d-electron systems (Cu and Au). The calculated spectral functions have been favourably compared with experimental results from the electron momentum spectroscopy group at AMPL. (A.S. Kheifets; F. Aryasetiawan [JRCAT, Japan])

The comprehensive investigation continues into the properties of magnetically ordered phases which appear in one- and two-dimensional strongly correlated systems, using the non-Abelian density matrix renormalisation group developed last year. In 1D, new ferromagnetic phases were discovered in the Kondo lattice and periodic Anderson models. In 2D, the stripes phase was studied in the tJ model. (M. Gulacsi and I.P. McCulloch; A.R. Bishop [Los Alamos National Laboratory, USA]; A. Rosengren and A. Juozapavicius [Royal Institute of Technology, Sweden])

The central problem posed by heavy fermion and collosal magneto-resistance (CMR) materials is to understand the interplay of localised moments and conduction electrons. In low dimensional, strongly correlated electron systems this problem was addressed using the Abelian bosonisation technique. The double-exchange ferromagnetic interaction was studied in the Periodic Anderson model. The impact of phonons on the magnetic properties of the Kondo lattice model was comprehensively analysed and the phase diagram of the model determined. The effect of the localised spin dilution was also studied in the Kondo lattice model. In this case, it was discovered that dilution drives the system to antiferromagnetism. (M. Gulacsi, P. McCulloch and H. Horn; A.R. Bishop [Los Alamos National Laboratory, USA]; A. Rosengren [Royal Institute of Technology, Sweden]; A. Bussmann-Holder [Max-Plank Institut, Germany])

The systematic investigation of the finite temperature properties of the Luttinger liquids continued. A finite temperature bosonisation method was developed and was consequently used to calculate all asymptotic correlation functions and critical exponents at any finite temperature. This result allowed the momentum distribution function to be calculated. Analysing the property of the momentum distribution the fractional statistics corresponding to the elementary excitations of a Luttinger liquid were established. (M. Gulacsi, G. Bowen and M. Parish)

At present the nature of high-temperature superconductivity remains elusive in spite of the fact that many novel models have been proposed. This problem was studied using a technique based on an infinite order unitary transformation. In theoretical physics unitary transformations are used to get deeper insight into physical phenomena, since the transformed Hamiltonians will reveal the appropriate independent subsystems. The transformation was successfully applied to the two and three band, 2D Hubbard models containing phonons. The effective spin and charge interactions were exactly determined. (M. Gulacsi and R. Chan)

Mesoscopic Systems

Charge conduction and current noise are intertwined phenomena. A unified description is made of both quantised conductance and nonequilibrium thermal noise in a 1D ballistic wire, open to macroscopic leads. While four-terminal measurements in such a conductor give evidence of resistance-free charge transport, its two-terminal resistance exhibits finite universally scaled quantised steps. On these results high-current noise offers a very different window. At the two probe conductance steps, the excess noise of field-excited ballistic carriers displays sharp peaks much larger than for shot noise. The thermal noise peaks are dramatically sensitive to the inelastic scattering effects in the leads that degrade universal conductance scaling. Thus, high-current thermal noise yields unique clues to the origin of contact resistance and the crossover to diffusive conduction. (M.P. Das and F. Green)

Applied research on a resonant soliton mechanism for ultrafast excitonic optical switching in semiconductors has continued. In particular, a wavelength dependence (effects of detuning) and a possibility of tunable operation of the resonant soliton switches and logic gates have been investigated. A fundamental difference in the response to detuning between a semiconductor nonlinear directional coupler (NLDC) and an atomic SIT-soliton NLDC has been revealed. A typical tunability range of a model resonant soliton NLDC has been assessed quantitatively and compared with a requirement for the device-operating spectral range in WDM systems (applied by the gain bandwidth of erbium-doped fiber amplifiers). An extensive literature search has been performed to identify semiconductor materials which are suitable for implementation of the resonant soliton switches capable of tunable operation near the optical communication wavelength (1.55 microns). A number of semiconductor systems with the required excitonic absorption features have been selected including InGaAs/InAlAs MQW, InGaNAs/GaAs MQW, InGaAs/InP MQW, InGaAsP/InP MQW and GaSb/AlGaSb MQW structures. Modelling of operation of InGaAs/InAlAs MQW NLDC near 1.55 microns has been performed. The ongoing research work is aimed at developing a new class of Tbit/s optical switches and logic gates for applications in ultra-high-capacity optical communication networks. The work has been funded by the U.S. Air Force Office of Scientific Research. (I. Talanina)

Atomic, Molecular and Nuclear Physics

Atomic Physics

Multiple atomic ionisation following absorption of a single photon or a knock out by a fast projectile is a dynamic, vibrant and controversial field of atomic collision physics. Because of the pivotal role of the electron-electron correlations, these processes continue to receive considerable attention, both theoretically and experimentally.

The close-coupling theory of the multiple atomic ionisation has been further extended. The role of various correlation mechanisms has been uncovered in double photoionisation of the helium atom. The cross-over between the shake-off and two-step mechanisms has been predicted theoretically and confirmed experimentally. The full parametrisation of the symmetrised double photoionisation amplitudes has been achieved offering a general description of the double photoionisation process at a very wide range of photon energies and geometries of the two-electron escape. The second-order corrections to the electron impact ionisation have been estimated in the double ionisation of the helium atom. (A.S.Kheifets; I. Bray [Murdoch University])

Quantum Chaos and Critical Phenomena in Finite Complex Systems

Anomalously strong sensitivity in finite quantum systems has been experimentally reconfirmed by the Beijing-Canberra-Lanzhou experiment-theory collaboration. By taking many repeat experimental points the absence of systematic errors in the series of the experiments was demonstrated. This provides the first experimental indication for the breakdown of quantum mechanics since quantum theory conceptually (in a model independent way) forbids sensitivity and chaos in finite systems. Yet the data support the new Kun theory of quantum chaos. Further tests of the theory will be carried out in China in 2002-2004 and in France in 2002. (S.Yu. Kun; Wang Qi et al. [Institute of Modern Physics, China]; Li Zhichang et al. [Institute of Atomic Energy, China]; F. Haas et al. [Louis Pasteur University, France])

The new Kun theory has been applied to calculate energy and time micro-channel cross-correlation functions for finite complex microscopic and mesoscopic systems. It was found that the micro-channel coherence undergoes non-equilibrium correlation phase transitions: initially the micro-channel coherence is absent and it switches on spontaneously by abrupt jumps at precisely defined moments of time. These results are in a sharp contrast with conventional theories where critical phenomena can be rigorously derived only in the thermodynamical limit, i.e. for infinite systems. For heavy-ion collisions the micro-channel phase transitions can be revealed from the high resolution energy dependence of the cross sections. In molecular and mesoscopic physics, e.g., for photo-disintegration of highly-excited polyatomic molecules and atomic clusters and fluorescence of quantum dots, the micro-channel phase transitions can be searched for by employing the standard experimental methods of femtochemistry. (S.Yu. Kun)

An alternative pedagogical explanation has been presented that Ericson fluctuations originate from the interference of randomly populated overlapping resonances. This explanation is important because of (i) the universality of Ericson fluctuations in a wide variety of fields, e.g., nuclear collisions, chemical reactions, coherent electron transport in nanostructures etc., and (ii) the significant role of Ericson fluctuations in the foundation of random matrix theory of open quantum systems. The present clarification is relevant in view of recent studies of electron-atom scattering where it was incorrectly claimed that Ericson fluctuations appear as a result of the absence of interference between randomly populated overlapping resonances. (S.Yu. Kun)

Antiproton-Deuteron Scattering

The experimental differential cross section for elastic scattering at 179.3 MeV has been fitted employing the scattering amplitude obtained from scattering experiments to determine the parameters of the elementary scattering amplitude at 179.3 MeV. The fitting was done using an analytic solution for the high energy elastic scattering amplitude obtained by employing a harmonic oscillator wave function with a D-state component for the internal wavefunction of the deuteron within the framework of Glauber's approximation to multiple scattering. The results have been compared with other analyses. (B.A. Robson; Zhang Yu-shun [Institute of High Energy Physics, China])

New Classification of the Fundamental Particles

A new classification of the fundamental particles (six leptons, six quarks and their twelve antiparticles) and the twelve fundamental 'force' particles (photon, three massive weak force bosons and eight gluons) based upon the use of only three additive quantum numbers (charge, particle number, generation quantum number) compared with the nine additive quantum numbers of the Standard Model (charge, electron lepton number, muon lepton number, tau lepton number, baryon number, strangeness, charm, bottomness, topness) has been proposed. The new scheme or Generation Model also differs from the Standard Model in that the hadrons are considered to consist of Cabibbo-Kobayashi-Maskawa 'mixed' quarks rather than the 'raw' or 'generation' quarks of the Standard Model. In this way the three additive quantum numbers are strictly conserved in strong, electromagnetic and weak interactions, unlike some of the quantum numbers of the Standard Model. (B.A. Robson)

Nuclear Fusion and Fission

The possibility of inducing the complete fusion of heavy nuclei has been a strong motivation in the quest to synthesise new nuclear species, especially superheavy elements. Work has commenced to develop a computer code using a semiclassical approach, incorporating conservative forces, dissipative (frictional) forces and fluctuating (Langevin) forces to calculate the probability of formation of a compound system for given target and projectile nuclei. It is also proposed to extend the computer code to describe the subsequent breakup, including fission processes, of the compound system. (B.A. Robson; G. Do Dang [Université de Paris Sud, France])

Nuclear Theory

Hadron Physics

A phase shift analysis of pion-nucleon scattering data at low energies has continued. The data base is very poor and criteria for the rejection of unsatisfactory experiments are being considered. (W.S. Woolcock; G.C. Oades [University of Aarhus, Denmark]; A. Gashi, E. Matsinos and G. Rasche [University of Zürich, Switzerland])

A calculation of the effect of vacuum polarisation on muon-proton scattering at small energies and angles has been made and published. (W.S. Woolcock; A. Gashi and G. Rasche [University of Zürich, Switzerland])

The influence of the hadronic interaction on the pionium wave functions has been calculated. A definitive study of the electromagnetic corrections to the scattering parameters obtained from experiments on pionium has been made. Both of these pieces of work are important for an experiment to measure the lifetime of pionium that is currently in progress at CERN. (W.S. Woolcock; G.C. Oades [University of Aarhus, Denmark]; A. Gashi and G. Rasche [University of Zürich, Switzerland])

Light Nuclei

Data for the 9Be(p, g)10B reaction with proton energies up to 1800 keV have been fitted using R-matrix formulae that include channel contributions. The data comprise values of the astrophysical S factor, branching ratios for transitions to the four lowest states of 10B, angular distributions and analysing powers. Information is obtained about six levels of 10B.

Values of the electron screening potential for various reactions between light nuclei are being obtained from fits to low-energy cross section data.

Measurements of the 14N(3He, 6He)11N cross section at eight angles covering 11N excitation energies up to several MeV are being analysed by R-matrix formulae in terms of the six lowest levels of 11N. (F.C. Barker; V. Guimaraes [University of Sao Paulo, Brazil])

Contributions to the two-proton decay of the second 1-state of 18Ne have been calculated, for comparison with recent experimental values. (F.C. Barker; B.A. Brown [Michigan State University, USA]); D.J. Millener [Brookhaven National Laboratory, USA])

Quantum Mechanics

Some interesting new results concerning uncertainty relations, fluctuations and information in quantum mechanics, have been obtained recently. Based upon these ideas it now seems possible to derive some basic equations of quantum mechanics in new ways. (K. Kumar and M. Hall)

The work on the scattering of electrons and ions from molecules continues to be of interest in relation to swarm theory. (K. Kumar, R. Robson; H. Skullerud [Institute of Technology, Norway])

High-Energy Physics and Cosmology

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

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