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Dublin Institute of Technology
Faculty of Science

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Final Year Projects in Physics

2002

Foreword

Welcome to the second edition of the DIT School of Physics graduates' yearbook. This publication presents the work that students have done in their final degree year research projects. They can be justly proud of their work and the School of Physics is pleased to be able to highlight their achievements in yearbook form. The projects represent the culmination of four years of training in experimental Physics laboratory work. Among the topics presented are Materials Science, Plasma Physics, Computational Physics, Quantum Mechanics, Electronics, Medical Physics, Molecular Materials, Acoustics and others. A brief personal description accompanies each student's project summary.

The students will now go on to the next phase of their careers. Physics graduates enter a wide range of careers, some of them apparently unrelated to Physics. They usually work in industry in a Physics, Computational or Engineering capacity, in research, or, in some cases in actuarial or financial services or teaching. One thing that all these careers have in common however, is the need to bring a creative approach to the solution of particular problems. The skills acquired in the study of Physics help to develop this approach to an exceptionally high level.

We do hope you will find this yearbook interesting and informative and that it will give some impression of the wide range of investigation undertaken each year by our students. If you would like to know more about our courses or the research activities of the School of Physics please visit our website at *http://physics.dit.ie* or telephone +353 1 4024559. The students can also be contacted through the School.

Dr Paul Horan
Acting Head of School
May 2002

Contents

The Measurement of the Light Output from a Variety of Medical Imaging Display Devices

Niamh Byrne
Supervised by Mr Tom Heary (Beaumont Hospital) &
Dr Tom Cantwell (DIT)

Personal Details

For my first three years in DIT Kevin Street, I studied the Diploma in Applied Science (Physics Option) and was awarded a Distinction. Upon graduating from the Diploma I was offered a place in the Applied Sciences Degree Course (Physics and Physics Technology). The subjects I have studied in my final year include medical imaging systems, biophysics, physics of materials, and optical communications.

During the summer of 2001 I worked in the DIT Facility for Optical Characterisation and Spectroscopy (FOCAS) as a research assistant, where I carried out research on detecting the presence of phenols in water using Raman spectroscopy. I also prepared Standard Operating Procedures for various spectrometers, including the UV/VIS and the FTIR.

Over the past five years I have held a part time waitress position and have spent two summers working in Canada and America. My interests include travelling and hiking and over previous summers I have travelled around Canada, America, and Peru where I got the opportunity to hike the Inca Trail and also in areas around the Grand Canyon, and the Rocky Mountains.

Project Summary

The purpose of medical imaging is to form an image of some part of the body in order to detect any abnormalities, which may or may not be present. There are many different types of imaging systems, such as radiography, Computed Tomography (CT), nuclear medicine, magnetic resonance imaging, and ultrasound. The display of the images produced by these systems is the final stage in the imaging process. Therefore the method of display and the quality of the display device affect the quality of the final image produced, which must then be interpreted by an observer.

There are two main display devices whose light outputs were investigated in this project. The traditional method involves imaging systems recording the images directly onto film. The film is then placed on a light-box, and may then be viewed by trans-illumination. With the advent of digital imaging systems, such as CT, display workstations were introduced. This allowed medical images to be viewed on cathode ray tube monitors. This digitising of medical images has made way for a Picture Archiving and Communications System (PACS) and also for a Teleradiology service. Figure 1 outlines this PACS.
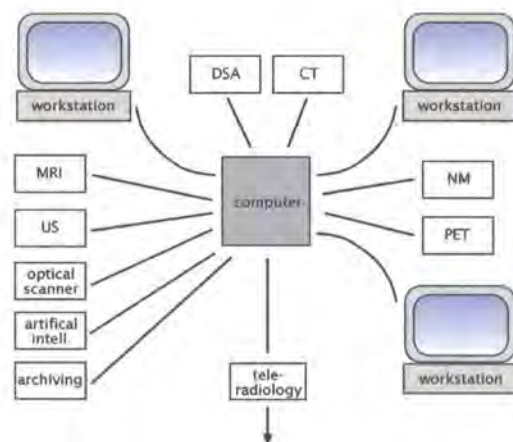

Figure 1: Picture archiving and communication system

PACS allows for the inexpensive storage of digitised images from all imaging systems. This

increases the speed and reliability with which images may be retrieved from storage, displayed on various workstations, and moved from place to place. Teleradiology allows the electronic transmission of images from one geographical location to another for the purpose of interpretation and /or consultation. Beaumont hospital is the centre for neurology in Ireland and its Teleradiology service is used nation-wide for consultation in relation to head injuries and neuro-surgical emergencies.

The two photometric quantities measured were *luminance* (SI units cd/m^2) which relates to the brightness of the display and *illuminance* (SI units lux) which relates to the ambient light. The luminance of various light-boxes at Beaumont was measured. The average luminance, the standard deviation, and the % variation for each was calculated. The department was then assessed as a whole. The results showed the average luminance to be 1660 kcd/m^2 and a variation of 26%. It is recommended by the American College of Radiology (ACR) that light-boxes have luminances within the range of 1340-4190 kcd/m^2, and the British Institute of Radiology recommend that luminances of light-boxes throughout the department should not vary by more than 20%. The average luminance for the department fell within the recommended range.

The digitising of images has also raised concerns regarding consistency in display. At the moment rigid standards exist for film but none yet exist for monitors. In 1986 the Society of Motion Picture and Television Engineers published a recommended practice for the evaluation of the performance of monitors. The most popular test pattern of this practice is the SMPTE pattern, shown in Figure 2.

Monitors were assessed using the SMPTE pattern. Their maximum and minimum luminances were measured and from this their luminance ratios were calculated, i.e. the ratio of the maximum and minimum luminance. This is an indicator of the response capability of the display with high luminance ratios indicating high quality displays. The ACR recommend a luminance ratio of 250. Our monitors ranged from 100-230.
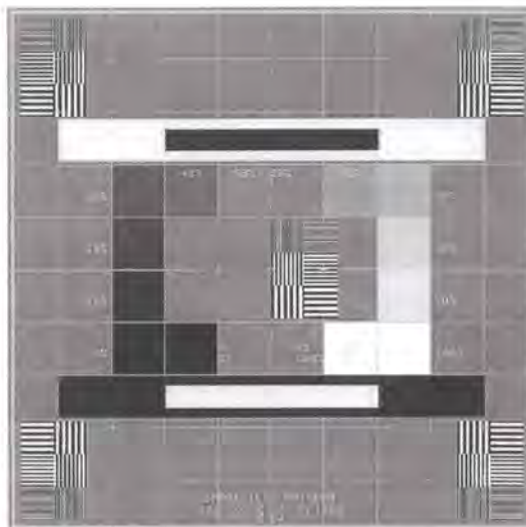
Figure 2. The SMPTE test pattern.

The Leeds test object was then used on fluoroscopy systems to determine the effect of ambient light on perceived image quality and spatial resolution. This test object consists of 14 discs of varying contrast and a resolution grid. The number of contrast discs that were perceived under varying conditions of ambient lighting was recorded. It was found that, with an illuminance of 266 lux, 11 contrast discs were perceived. However, when this was reduced to 26 lux, 12 contrast discs could be seen and when ambient light was reduced to a minimum, 13 contrast discs were visible. Ambient light was not found to have any significant effect on perceived resolution.

In conclusion, recommendations were made for the regular assessment of all light-boxes in the department, as well as the cleaning and replacement of light-boxes that fell outside the range recommended. For monitors, it was recommended that the luminance ratios be set to the same values in order to maintain consistency in the display of images when viewed at different monitors. It was also recommended that the ambient light be reduced to a minimum around monitor viewing stations, as it has a more significant affect on monitors due to their lower luminance capabilities.

The Interaction of Carbon Nanotubes with Supramacromolecules

Clodagh Carroll
Supervised by Dr Gordon Chambers

Personal Details

In 1999, I successfully completed the Technician Diploma in Applied Sciences (Physics option) with grade Merit 1. Having been afforded the opportunity, I decided to further my studies by transferring into the Degree in Applied Sciences (Physics & Physics Technology option).

During my time in DIT Kevin Street I acquired several skills including report writing, presentational skills and teamwork as well as computer skills including C programming, MATLAB, Excel and Powerpoint.

Before beginning my degree I worked in FOCAS at DIT as a research assistant for 3 months. After this I spent 6 months working in New York. I've also travelled extensively in Europe and America throughout my college career and on completion of my degree I look forward to travelling in Peru.

Project Summary

Since the discovery of carbon nanotubes in 1991 by Japanese electron microscopist Sumio Iijima, there has been considerable interest in their development. The motivation for research in the area of carbon nanotubes is primarily to revolutionise electronic technology, as nanotubes can be considered as prototypes for one-dimensional building blocks for nanoscale devices.

Carbon nanotubes are fullerene-related structures, which are unique for their size, shape and physical qualities. Essentially a carbon nanotube can be thought of as being a sheet of graphite, (a hexagonal lattice of carbon), which is rolled into a cylinder and closed at either end with caps containing pentagonal rings, as shown in Figure 1. Two different classes of nanotube exist, small diameter, single-wall nanotubes, (SWNTs, $\approx$ 1nm) and large diameter multi-wall nanotubes (MWNTs, $\approx$ 10nm). SWNTs can be thought of as the fundamental cylin-

drical structure, and these form the building blocks of both multi-wall nanotubes and the ordered arrays of single-wall nanotubes called ropes. Multi-wall nanotubes, as the name suggests, contain several concentric tubes of carbon, nested inside each other. It has been proposed that carbon nanotubes possess remarkable electronic and mechanical properties. However, a major obstacle with the development of carbon nanotubes is that it is difficult to process them.

In this study the intermolecular interactions of small diameter SWNTs and large diameter MWNTs with a supramacromolecule, γ-cyclodextrin were examined as a method of dispersion. It is proposed that γ-cyclodextrin may help in achieving the processability of carbon nanotubes as it is known to be capable of forming complexes with other carbons such as C_{60}, therefore facilitating chemical manipulation.
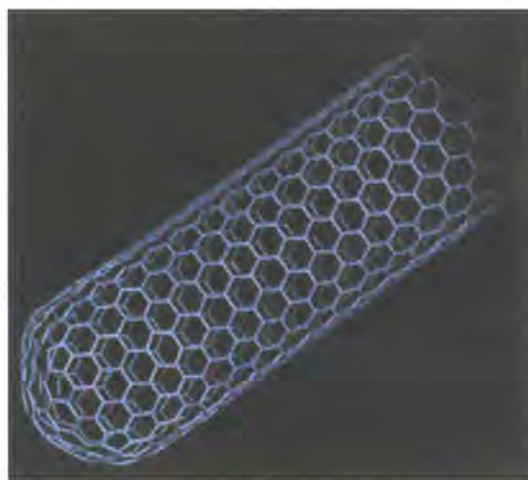
Figure 1. Model of the typical SWNT structure

The two milled samples were prepared by grinding the tubes and γ-cyclodextrin in a 1:30 ratio together in the presence of ethanol until a fine, black homogeneous powder was obtained. The pristine samples and the milled samples were characterised using absorption spectroscopy, Raman spectroscopy, Differential Scanning Calorimetry (DSC) and Transmission Electron Microscopy (TEM).

It was found that SWNTs do interact with γ-cyclodextrin by inducing a compressive strain along the length of the tube. This was observed by the significant shift of the G-line and the RBMs in Raman spectra. A notable change in shape and position in the DSC scan from the pristine form also gave strong indication of interaction using thermal analysis. Finally, TEM images such as shown in Figure 2 provided direct confirmation that the SWNTs were successfully dispersed away from their characteristic bundles due to the addition of γ-cyclodextrin.

Using the same analysis, no evidence was obtained to suggest that MWNTs interact with γ-cyclodextrin. The spectra that are normally susceptible to changes in the environment did not undergo any deviation from their characteristic positions. This implied that the interaction of γ-cyclodextrin with carbon nanotubes was diameter dependent

It was concluded from spectroscopic evidence that γ-cyclodextrin interacted with SWNTs by adsorbing to the side of the tube through the van der Waals force and thus applying a strain along the length of the tube. This interaction would not be strong enough to have an effect on the larger diameter of the MWNTs and so no interaction was detected.
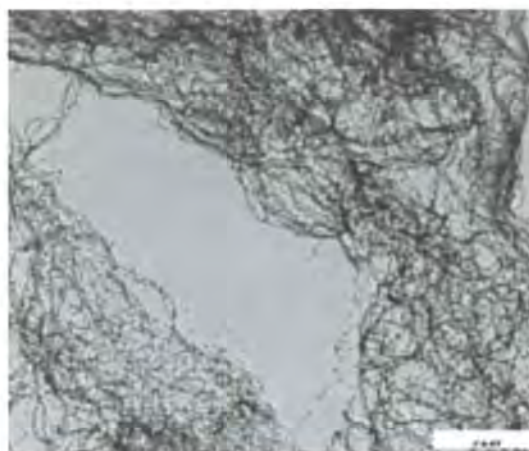
(a)
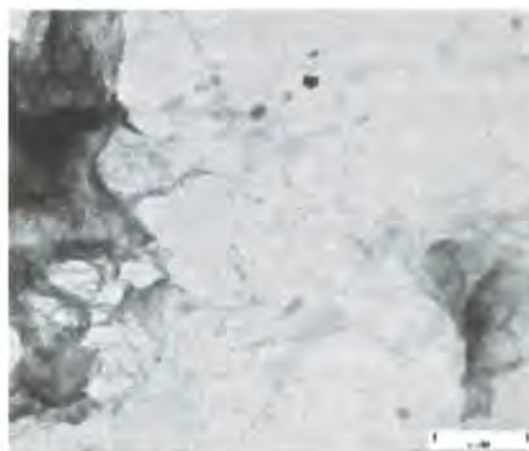
(b)

Figure 2. TEM image of (a) raw SWNT and (b) SWNT/ cyclodextrin milled compound.

Investigation of the Chaotic Dynamics of an Electronic Analogue of the Duffing Oscillator

Pat Chambers
Supervised by Dr Cathal Flynn

Personal Details

Upon completing a Diploma in Instrumentation and Applied Physics at the Institute of Technology, Tallaght, I transferred onto year three of the BSc in Physics and Physics Technology at DIT. In my final year I took options in Microwave engineering, Acoustics, Optical Communications and Fluid Dynamics. As a result of doing this project I became interested in undertaking scientific research. I would like to continue in the area of chaos theory or undertake communications based research. I am a keen swimmer and have won medals for the Institute of Technology, Tallaght. As well as this I enjoy listening to and playing music, particularly the Blues.

Project Summary

Chaos is a word which describes systems whose behaviour is unpredictable. Both simple and complex systems can behave chaotically given the right parameters. Chaotic systems are sensitive to initial conditions. This causes a problem when we try to predict their behaviour for all time. In order to predict the weather, a very familiar system, we would have to know the state of the atmosphere at present to a degree of accuracy that is not possible by modern methods. The weather is a chaotic system. The effect of a very small difference between the known state of the system and the actual state of the system is amplified over time. Chaotic systems exhibit non-periodic behaviour in that they never repeat their exact motion. Their behaviour can, however, stay within limits known as a "strange attractor". For example the weather in some hot countries can give temperatures as high as 50 ^{0}C but never lower than 30^{0}C. These limits are the strange attractor for the weather in these countries.

The Duffing oscillator is a non-linear system that can exhibit both a periodic and a chaotic response. It is a damped, driven oscillator. It is modelled by a non-linear, second order differential equation

known as the "Duffing Equation". The Duffing equation for the system in Fig. 1 is

$$m\ddot{x} = kx - kx^3 - \alpha\dot{x} + A\cos(\omega_0 t)$$
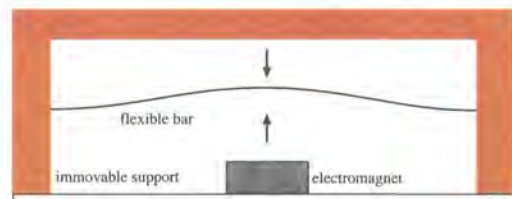
Figure 1. The Duffing oscillator set-up shows the driving electromagnet coupling a flexural bar.
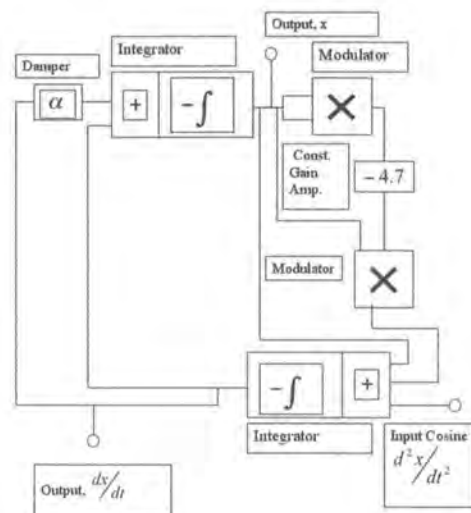
Figure 2. Block diagram of electronic analogue of the Duffing Oscillator which models the Duffing equation.
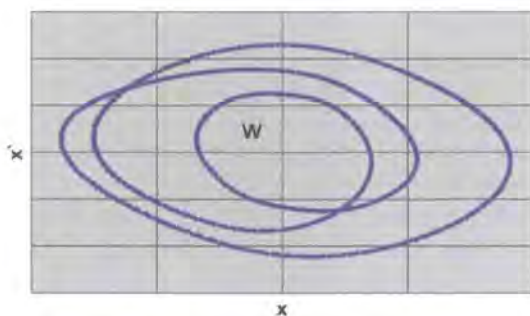
Figure 3. Observed period three behaviour from the Duffing Oscillator circuit.
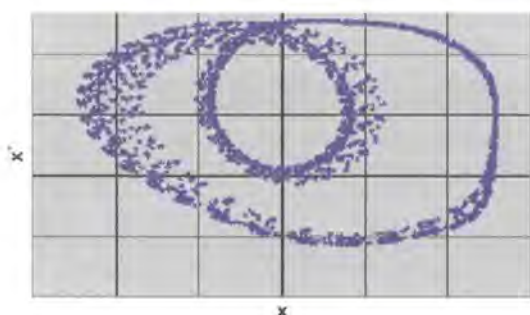
Figure 4. Observed chaotic behaviour from the Duffing Oscillator circuit

This equation cannot be solved by simple Laplace methods; instead we must solve it computationally. The purpose of this project was to build an electronic circuit that models the Duffing equation and observe its behaviour for different parameter values of driving and damping. A block diagram for the circuit is presented in Figure 2.

The circuit gave us multiple periodic behaviour and, as well, what we believed to be chaotic behaviour. The circuit was analysed in phase-space, which corresponds to X-Y mode on an oscilloscope. This allowed us to see periodicity quite clearly.

Period three behaviour was observed (Figure 3) and it has been shown mathematically that this implies that for certain system parameters, there will be chaotic behaviour. Dataplore was used to try and determine whether the behaviour was chaotic or not, as it could have been multiple period. It was a student edition so its authors purposely limited its capability; it therefore only indicated chaotic behaviour (Figure 4).

I found this project very challenging, both in terms of its electronics content and in getting to grips with understanding chaos theory. It has, however, been a very rewarding experience. Chaos theory has caused me to see the scientific method in a whole new light. I am keen on doing research in this area.

Comparison of the Resonant Frequencies of Real and Computer-Simulated Soundboards

David Charles
Supervised by Patrick Healy

Personal Details

For the first two years of the BSc course I studied Physics, Computer Science, Mathematics, Management Studies and Spanish. In third year I switched course to study Physics Technology instead of Computer Science. My final year subjects comprised Physics and Physics Technology and in particular I chose to study Microwave Engineering, Optical Communications and Acoustics from Physics, and Information Processing and Biophysics from Physics Technology. I am interested in scientific research and development in areas such as the Communications Industry, Computer Industry, Biological Engineering and Lasers. My hobbies include listening to and producing music and playing football.

Project Summary

My project involved the comparison of resonant frequencies from a computer-simulated harp soundboard with the resonant frequencies of a real soundboard. The soundboard was modelled using ANSYS, which is an engineering software tool that allows for the construction of a model and the application of physical conditions to it. A model of the soundboard was built and a vibration analysis was performed yielding the computed resonant frequencies of the model. The real soundboard was then set up to have vibration analysis performed on it. With the use of various tools including transducers, sampling units and Fast Fourier Transform (FFT) software, the apparent resonant frequencies of the soundboard were calculated.

ANSYS is a Finite Element Analysis (FEA) software package, which is used to produce accurate approximations of real systems. A real physical structure is composed of a large number of very small elements. To model a structure perfectly, each of these tiny elements would have to be accounted for. This would take far too long to do even with the fastest computers. The Finite Element method breaks a large physical structure down into many smaller segments. Each of these smaller segments can be modelled using a computer and when analysed, can then be convolved to reproduce solutions for the model as a single structure. Results for the model were in both tabular and graphical form. The graphical form gave extra information about how the soundboard would look during vibration (Figure 1).
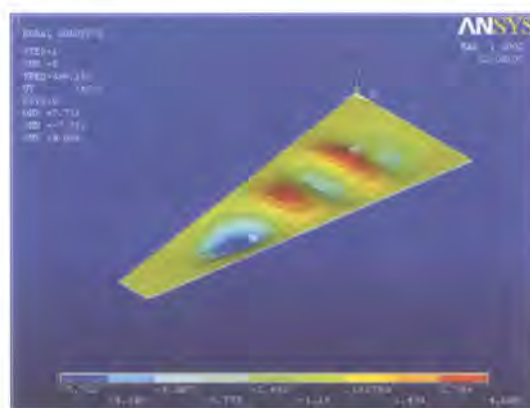
Figure 1. ANSYS model of soundboard

The real harp soundboard was then subjected to testing. The system used to perform the test was an amalgamation of different tools. An accelerometer, which was used to measure the vibrations on the surface of the soundboard, is a transducer that converts acceleration into an electric signal. The electric signal was then relayed to the Strobes Acquisition unit. This unit is used for sampling electrical signals and then converting this to a digital format. The signal produced by the accelerometer was analogue (continuous) in nature. The
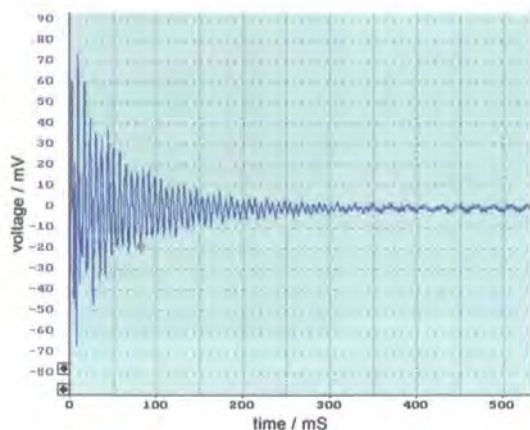
Figure 2. Time spectrum of soundboard vibration

Figure 3. Frequency spectrum derived from Figure 1.

unit records the level of the signal at regular time intervals and creates a list of these levels and the times they occurred. A rate of 5000 samples per second was used in my project. The data was stored in the unit until enough samples had been taken to form a complete picture or frame of the signal. The frame was then sent to a computer for FFT analysis. The FFT software showed a visual representation of the signal (Figure 2). The software could apply the FFT algorithm to the digitised data to display a frequency spectrum of the signal data. This allowed the signal to be seen as the sum of its frequency components (Figure 3) from which the frequency values were recorded.

The simulated and real frequencies were compared against each other to gauge the accuracy of the computer simulation. Due to various factors, the frequencies were dissimilar so a new way of comparing the recordings was used, which compared the ratios of the frequencies to their respective fundamental frequencies. The modes of vibration could be seen in the computer output (Figure 1).

The modes of vibration were not seen on the real soundboard although there are various techniques to do this including laser vibrometers and the Chladni powder method (sprinkling a powder on the board and watching its movements).

The project contained a good mix of theory learned during the course, and practical work, which made it enjoyable to work on.

The Application of Spectroscopy in the Analysis of Biological Samples

Jennifer Conroy
Supervised by Dr Hugh Byrne & Dr Fiona Lyng

Personal Details

I completed a three year Diploma in Applied Physics in DIT Kevin Street, during which time I was awarded a scholarship from Intel. Following on from the Diploma I was offered a place in the Applied Sciences Degree Course (Physics and Physics Technology). During the summer of 2000 I worked in Tallaght Hospital and was assigned to the BioEngineering Department, following a project I had completed during my Diploma with the ICU Department. During the summer of 2001 I was employed as a research assistant by the DIT FOCAS facility. While working there I gained a lot of practical experience, especially in the area of spectroscopy. This is where the interest for my project stemmed from.

I am interested in travelling and spent the summer of 1998 in Cape Cod on a J1 visa. When I finish my Degree I hope to travel the world for a year; after that perhaps I may further my studies. I am also interested in all kinds of sports especially soft-ball and hockey. Other interests include swimming, mountaineering and of course socialising.

Project Summary

Sadly today cancer is a disease that all of us have faced either directly or indirectly through our family and friends and so on. Cancer is the leading cause of death in the western world. The key to the successful treatment of cancer is primarily early diagnosis. More often than not, if this disease is diagnosed in the early stages it can be treated which increases the chances of survival and sometimes a full recovery.

As scientists we are fortunate to have the opportunity to work in such areas as allowing for the development and improvement of techniques such as the diagnosis of cancer. At present, cancer diagnosis involves the analysis of a piece of tissue from a biopsy by a pathologist. This involves the evaluation of the tissue sample using microscopy. The morphology of the sample is examined leading to diagnosis. This particular method of diagnosis is invasive and time consuming. The tissue sample to be analysed has to be processed into paraffin wax blocks, sectioned using a microtome and stained. This prolongs the diagnosis for a patient, which can lead to a great deal of stress. Ideally the possibility of real time diagnosis would save money, time and the anguish for a patient, thus leading to the push toward *in-vivo* diagnostics.

In-vivo diagnostics would lead to real time results, which is where the potential of spectroscopy comes into play. The human body is composed primarily of water, proteins, nucleic acids, lipids and carbohydrates. Any changes in the body leading to diseases such as cancer are thought to be due to some biochemical changes in one or all of these components. If spectra are sensitive to the structure of these components, then the spectra would be expected to change with the diseased state also. In this project, proteins and nucleic acids were studied using spectroscopy.

Three methods of spectroscopy were employed to analyse these biological samples, UV/VIS absorption spectroscopy, fluorescence spectroscopy, and Raman (vibrational) spectroscopy. From these, Raman spectroscopy proved to be the most suitable method for the analysis of biological samples.

Unlike a biopsy, where whole cells and tissues are analysed, this study entailed the analysis of the constituent components of proteins and nucleic acid (DNA). Spectroscopy was used to analyse amino acids (the constituent components of pro-
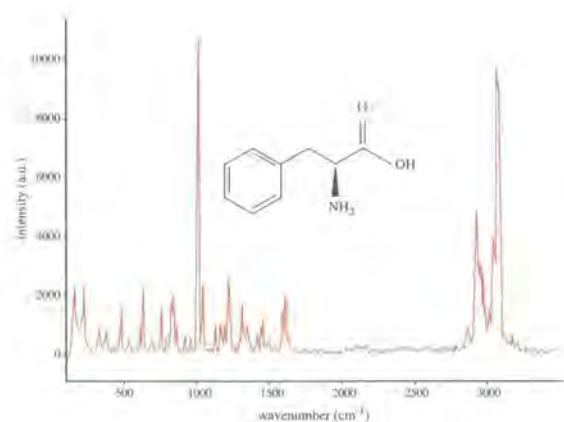
Figure 1. Raman spectrum of the Amino Acid Phenylalanine and the phenylalanine molecule. The peak at 1004 cm^{-1} corresponds to the benzene ring in the molecule.
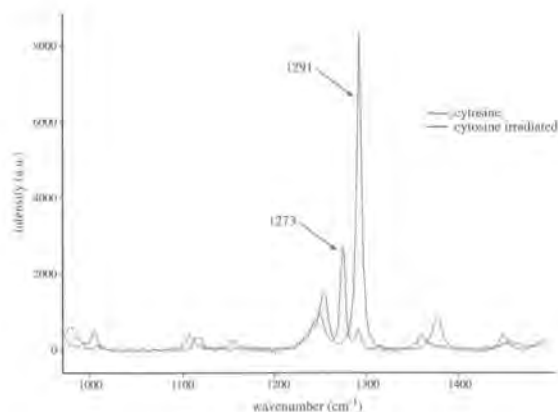
Figure 2. Raman spectra of Cytosine powder and irradiated cytosine. The peak at 1273 cm^{-1} disappears after radiation whereas there is a huge increase in the peak at 1291 cm^{-1} after radiation.

teins and peptides) and the purines and pyrimidines (the constituent components of nucleic acids). This was carried out with the aim of creating a library of spectra that are individually characteristic to each biological sample to be analysed. It was also hoped that the constituent components would be identifiable in the more complex structures i.e. the peptides, proteins and DNA. One further expected the signature of these components to be traceable on a cellular level, thus providing standard spectra for comparison with those of samples that are diseased or irradiated.

As mentioned above the spectra of the constituent components were expected to change with the diseased state. This is due to biochemical changes within the sample. In order to mimic that of a diseased state a number of samples were irradiated with ionising radiation. The radiation caused bio-

chemical changes in some of these samples. The spectra of the irradiated samples were then compared to those of the "healthy" or standard samples.

A number of significant differences were observed between the Raman spectra of cytosine (pyrimidine) and irradiated cytosine. There were also a number of significant differences between the Raman spectra of glutamic acid (amino acid) and irradiated glutamic acid.

All the Raman spectra observed provided characteristic peaks that were unique to the sample in question. The signatures of the constituent components proved to be partially traceable in the more complex protein and DNA structures. There were striking similarities between the Raman spectra of the peptides and proteins. This is due to their similar backbone structure made up of peptide bonds.

Investigation of the Freedericksz Transition in Liquid Crystals

Michelle Conway
Supervised by Elizabeth Gregan

Personal Details
In my first three years in DIT Kevin Street, I studied for the Diploma in Applied Sciences (Physics Option) and was awarded a Merit 2. After graduating I was offered a place in the Applied Sciences Degree course (Physics and Physics Technology). The subjects I studied included medical imaging, material science, microwaves and nuclear physics.

During the summer of 2001, I worked in the medical centre for Guinness at James Gate, Dublin. At Guinness I was involved in local community work, and awarded school children Certificates of Merit for attending school. I also attended other similar functions, as Guinness takes a big interest in the welfare of the community around it. During other summer holidays I worked for Irish Rail. My interests include travelling, and kick boxing. When I leave college I would like to go to New York, and then travel through Europe.

Project Summary
The aim of my project was to reproduce the Freedericksz Transition in a liquid crystal and show the dependence of the Freedericksz Transition threshold on the inverse sample thickness. The paper on which this work was based was written by T. Mosses and J. Jensen "*The investigation of the Freedericksz Transition in liquid crystal for an undergraduate laboratory.*"

The Freedericksz Transition occurs when there is competition between elastic and magnetic forces on the liquid crystal. If a magnetic field is applied to the crystal then the magnetic dipole moments are induced in the molecules. This causes the molecules to align along the magnetic field. This does not occur at the surface of the molecule, due to strong interactions within the substrate molecule that keeps them fixed. Reorientation takes place in the rest of the crystal along the field direction. This entails a distortion in the direction of the molecules. This distortion costs energy just as the deformation of any elastic medium requires energy. When the applied magnetic field H is greater than a threshold value H_o then reorientation occurs. If the magnetic field H is less than this threshold then no reorientation occurs. This is so because when the magnetic field $H < H_o$, the energy reduction due to the magnetic poles reorienting is outweighed by the energy cost of the elastic deformation. When $H > H_o$, then it is energetically favourable for the molecules to reorientate despite the elastic energy cost. So therefore as the magnetic field increases beyond a threshold value, the Freedericksz Transition occurs. The threshold is seen when $H/H_0 = 1$.

There are three primary deformations of a nematic liquid crystal, known as the splay, twist, and bend. These are shown in Figure 1. The splay elastic constant is calculated from the following equation:

$$H_0 = \pi / d \left[K_1 / \mu_0 \Delta\chi \right]$$

where H_0 is the threshold field, d is the spacer thick-
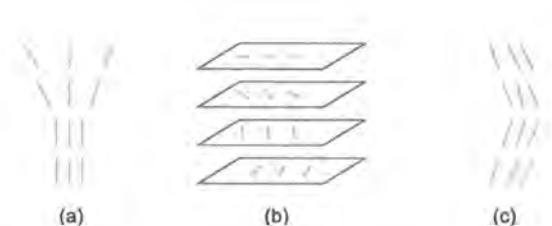
Figure 1. Primary liquid crystal deformations (a) splay, (b) twist, (c) bend.

Figure 2. Apparatus showing laser (left) followed by polariser and magnetic poles (right)

Figure 3. Initial phase shift versus H/Ho for 177.8 µm

ness used to put in between two glass slides when forming the liquid crystal cell, μ_0 is the permittivity of free space, χ is the magnetic susceptibility and K_1 the splay constant.

A large splay constant K_1 increases the energy cost of deformation, raising H_0. Large magnetic susceptibility anisotropy makes reorientation more energetically constructive, decreasing H_0. A smaller sample thickness d decreases the distance over which the director must deform, raising the elastic energy cost and increasing H_0. According to the above equation, the Freedericksz Transition threshold field H_0 is inversely proportional to the sample thickness. This can be shown graphically which results in a straight-line graph.

To achieve this transition, the liquid crystal sample was placed in between two magnetic poles. A laser beam was passed through a polariser, through the first axial hole in the magnet, through the liquid crystal, through the second axial hole in the magnet, through a second polariser and then focused onto a photodector (see Fig. 2). The polarisers were crossed, with one of the polarisers parallel to the optic axis (nematic director) of the sample. The second was then adjusted so that minimum transmission was achieved. Five liquid crystal cells were made up with spacer thickness of 25-250µm.

Figure 4. Experimentally derived Freedericksz Transition threshold field Bo versus inverse sample thickness

The results, illustrated in Figures 3 and 4, concurred quite well with the expected behaviour of the Freedericksz Transition, particularly for phase shift versus field ratio. Some deviation from the expected linear relationship between threshold field and sample thickness was observed.

Investigation of The Wigner Function and Quantum Entanglement

Gerard Duff
Supervised by Dr Michael Tuite (School of Mathematical Sciences)

Personal Details

I came to DIT Kevin St. in 1995 to study physics and mathematics. Having completed 3 years of the BSc (Applied Sciences) course, which included courses in management studies and German, I was sidelined for personal reasons for a further 3 years. I made a return to college in September 2001 for my final year. I have thoroughly enjoyed my time in the DIT and have found life in Kevin St. quite easy to adjust to, even the second time around. I am interested in all aspects of mathematics, applied mathematics and physics and in the teaching of those subjects.

Project Summary

My final year project, proposed by the School of Mathematics, is mathematical physics based. I was concerned primarily with a probability distribution function called the Wigner function, (Eugene Wigner 1932), a version of which has applications in a range of quantum technologies including quantum optics and quantum computing. The aims of the project were to (i) carry out a study of the Wigner function $W(p, q)$ and its properties, (ii) to investigate some of its applications to, for example, coherent and entangled states of light.

I began by studying the elements that make up the Wigner function itself. Those elements are, phase space, Fourier transforms, and the density matrix. Phase space means simply position and momentum space. Many physical situations lend themselves to analysis in phase space; e.g. Heisenberg's Uncertainty Principle $\Delta p . \Delta x \approx h/4\pi$ is an expression in phase space, which is fundamental to physics. The density matrix is a very powerful tool in applied maths. Knowledge of the density matrix gives a full picture of the state of the entire system as a statistical or 'ensemble' average. The version of the density matrix used here also contains information about quantum expectation values. It also allows us to predict the value of an arbitrary observable **A**, by
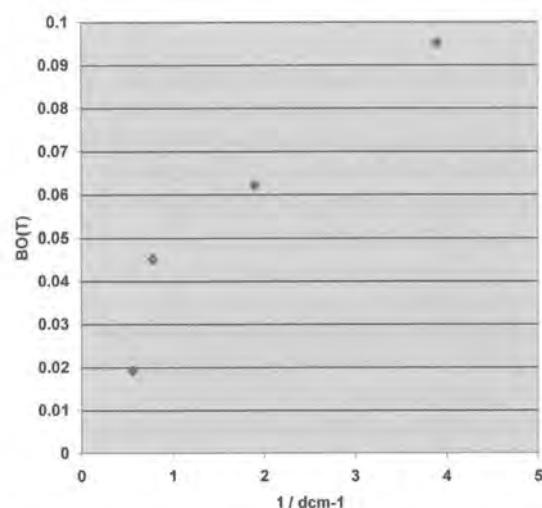
means of the commutator $[\hat{A}, \rho]$.

$W(p, q)$ is a Fourier transform, and is given by Equation (1) below. Its inverse transform is given by Equation (2).

$$W(p,q) = \int_{-\infty}^{\infty} dr \exp(-ipr/\hbar)\langle x|\hat{\rho}|x'\rangle \tag{1}$$

$$\langle x|\hat{\rho}|x'\rangle = \overline{\psi(x)\psi(x')} = \frac{1}{h}\int_{-\infty}^{\infty} dp \exp(ipr/\hbar)W(p,q) \tag{2}$$

The Wigner function gives a full description of the state of the system in terms of $|\psi(x, t)|^2$ where $\psi(x, t)$ is the solution to the time dependent Schrödinger equation. In this way the Wigner function has been used to reconstruct $|\psi(x, t)|^2$ for
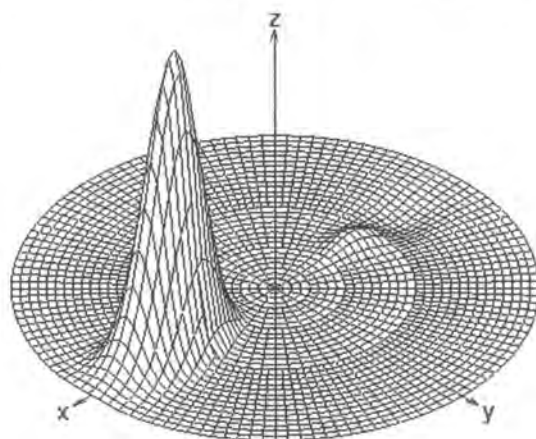
Figure 1. An example of the Wigner function where the x-y plane corresponds to the phase plane (p, q), and the z-axis corresponds to W(p, q).

many different quantum states.

One such state is known as a *coherent state*. Coherent states are regarded as being quasiclassical. For example, a coherent state harmonic oscillator is analogous to the motion of a pendulum. The particle or wave of finite length is said to *cohere*, in the sense that it sticks together.

Figures 1 and 2 are graphs of two possible Wigner functions, where the x-y plane corresponds to the phase plane (p, q), and the z-axis corresponds to $W(p, q)$.

The Wigner function of a coherent state (Fig.1) is a Gaussian bell curve and is positive everywhere. Such a state is called a minimum uncertainty state or M.U.S. Such states hold a special place in quantum mechanics, since they give an "equals to" in Heisenberg's relations.

An entangled state (Fig.2) however has negative fringes in its Wigner function. This is due to 'interference terms' which appear in $W(p, q)$. For example, the Wigner function of Young's double slit experiment is similar to Fig.2. The interference terms have no classical analogue. It is for this reason that the magnitude of any negativities in the Wigner function are indicators of, and used to explore the so called classical-quantum boundary.
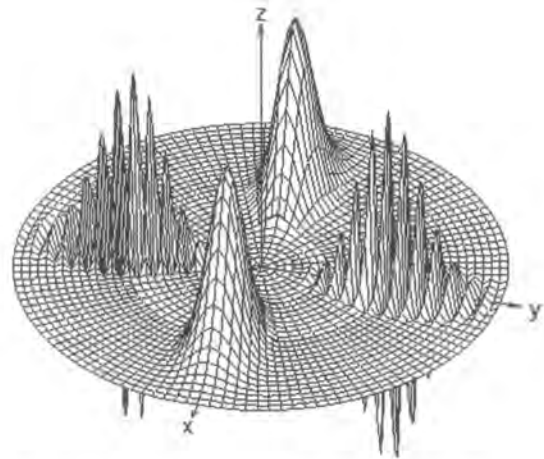
Figure 2. A further example of the Wigner function where the x-y plane corresponds to the phase plane (p, q), and the z-axis corresponds to W(p, q). Interference terms in the Wigner function produce the characteristic peaks similar to what is observed in a Young's double slit experiment.

The Wigner function is called a *quasiprobability distribution function* because of the presence of these negative values.

The project deals with entanglement in a more mathematical way, via what is referred to as a *tensor product*, also the idea of a quantum bit or qubit is discussed.

The Spectral Characterisation of Plasma Deposition Processes

Sinead Egan
Supervised by Dr Denis Dowling & Dr Miriam McConnell
(Enterprise Ireland) and Dr Des O'Mahony (DIT)

Personal Details

After successfully completing three years at DIT Kevin Street, I was awarded a Diploma in Applied Science (Physics Option) with a Merit 1 Grade. To further my education, I transferred to the Degree in Applied Sciences, Physics and Physics Technology Option at DIT.

For my final year projects in each course I attended the Surface Engineering Laboratory at Enterprise Ireland where I was afforded the opportunity to study thin films and the plasma state. Before undertaking the final two years, I worked in FOCAS at DIT Kevin Street for nine months as a research assistant and also travelled extensively throughout the U.S.A. My interests include swimming, travel and socialising.

Project Summary

Plasma deposition has been extensively used for the fabrication of thin films with a wide range of technological applications. Despite the practical success, much remains to be understood concerning the detailed processes in film forming discharge of organic gases.

Plasma Optical Emission Spectroscopy (OES) has been recognised to be an efficient tool for plasma diagnostics and for the monitoring of chemical species present within the plasma processes used for thin film deposition. Particularly, the OES technique is a powerful method for the '*in-situ*' diagnostic of the complex processes occurring in the glow discharge. Among the advantages that this sensitive detection technique offers is its high space resolution and the fact that it allows real-time information on the processes in the plasma without producing any interference with them.

In this study, an argon plasma, used to sputter a Ti target in a magnetron sputtering system, was monitored '*in-situ*' by means of an OES technique.

The relationship between the relative intensity of emission lines is a complicated function of the sputtering conditions (pressure, target current, gas flow) as well as the geometry of the target. Plasmas are a glow discharge phenomenon, the colour and wavelength of which is specific to various gases and elements within the plasma (for example, an argon plasma appears blue and a nitrogen plasma appears pink). OES monitored the intensities of various species within the plasma because intensity was indicative of concentration of that species. In magnetron sputtering, two different species were present in the plasma which were the argon, and the titanium plume emanating from the target. Therefore it was possible to monitor both plasma and deposition simultaneously.

The aim of this study was to use OES to monitor the plasma. In this way the optimum conditions that favoured the growth of thin films were determined. Films were grown on stainless steel substrates and evaluated using four different test methods. A direct correlation was established between emission peak-
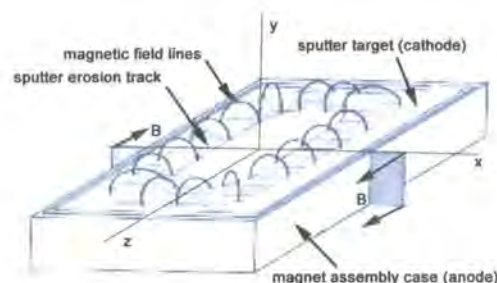
Figure 1. Schematic of the magnetron configuration for optimised sputtering

intensity with target current and with pressure. In this study, it was found that the concentration of argon increased linearly with pressure and with target current. Two argon peaks were monitored over varying pressures and targets currents.

Similarly with Titanium, two peaks were again monitored, 508nm and 522nm. Both emission peaks increased linearly with both pressure and current.

Optimum conditions that favour the growth of thin films were found at a pressure of 3×10^{-3} mbar and a target current of 2.5 Amps. These parameters were chosen because at lower pressures, and higher currents, there was a higher concentration of both argon and titanium in the chamber and a greater probability of collision taking place, therefore a higher deposition rate was expected.

This was confirmed when the coatings were evaluated. A Titanium Nitride (TiN) coating was deposited on a stainless steel substrate with the above parameters. The coatings were evaluated using four different test methods - adhesion, friction, hardness and film thickness. The films exhibited excellent friction, adhesion and hardness properties.

The table below compares properties of the film to the properties of the substrate:

	TiN	Stainless Steel
Friction	0.55	0.7
Adhesion	HF1	------------
Hardness	1936HK	1307HK

Preservation of the Structural Integrity of Modified Phases of C60

Colm Faherty
Supervised by Dr Gordon Chambers & Dr Hugh Byrne

Personal Details:

After successfully completing three years study at DIT Kevin Street, I was awarded a Diploma in Applied Science (Physics Option). To further my education, I then transferred into a degree course in DIT in Physics and Physics Technology. Over the past five years in college I have maintained different part-time jobs, as well as working in America for a period and have continued involvement in many other activities outside the academic field. I have played inter-county football and hurling as well as competitive soccer. Other hobbies include boxing, socialising and travelling out of which I hope to travel around Australia for a few months after I graduate.

Project Summary

The C_{60} molecule, or Buckminsterfullerene, was discovered in 1985 and has been shown to be both photochemically and thermally unstable in the solid state at room temperature. However, below room temperature the C_{60} molecules rearrange themselves in the lattice to a much more stable state. It was the aim of the project to achieve this stable state at room temperature, through the use of three techniques: solvent inclusion, annealing and a combination of annealing and solvent inclusion. The results of each technique were analysed using electron microscopy, vibrational spectroscopy and Differential Scanning Calorimetry (DSC). If a stable lattice can be achieved, it is proposed that the C_{60} molecules can be manipulated for electronic purposes. Solvent inclusion involved exposing the C_{60} film to chloroform in a petri dish for a total of 3 hours while annealing involved heating the C_{60} film in a vacuum oven for 48 hours. It follows then that the combination process involved heating the film and then exposing it to chloroform.

Optical absorption showed the results of each technique to be very similar. There was no change in the HOMO-LUMO (highest occupied molecular orbital – lowest unoccupied molecular orbital) peak at 630nm indicating that the system was still molecular in nature, while there was considerable loss of oscillator strength at 450nm. This peak is attributed to the solid state features of the molecule, so a loss in strength indicates that the packing in the lattice has changed (see Figure 1).

Raman spectroscopy revealed pure C_{60} to have a mode at 1469cm^{-1} which was unstable to prolonged illumination (see figure 2). With each technique used, Raman spectroscopy revealed dramatic differences. With Solvent Inclusion the 1469cm^{-1} mode shifted to 1464cm^{-1} and remained stable to prolonged illumination. There was also a new feature at 1459cm^{-1}. The annealed film contained 2 peaks, the 1469cm^{-1} mode and a new feature at 1464cm^{-1} which was partially stable to prolonged illumination. The best result was achieved with the
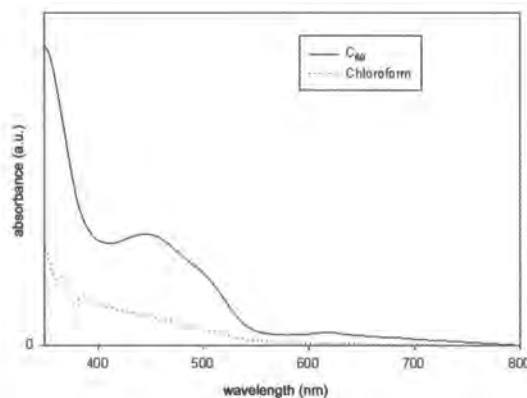

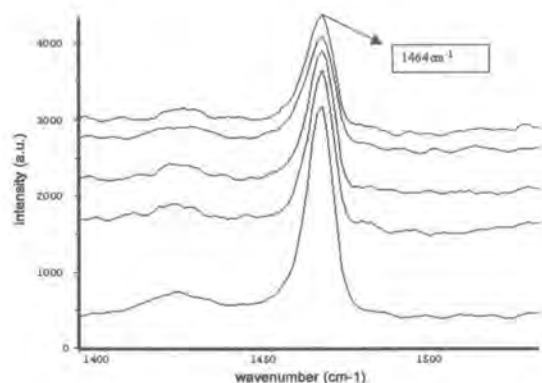*Figure 1: UV Analysis of C_{60} film exposed to Chloroform*

Figure 2: Raman Analysis of C_{60} film

Figure 3: Raman Analysis of Annealed and Exposed film

combination process which showed a shift of the 1469cm^{-1} mode to 1464cm^{-1} and this new feature remained stable to prolonged illumination, with no appearance of any new feature (see Figure 3). This indicates that the structure of the lattice has changed to a much more stable state. Most importantly, using microscopic analysis, the surface of each film was analysed and it was found that with solvent inclusion, the surface was ruined while the annealing process helped retain the surface integrity. The combination process partially retained the surface integrity and with Raman spectroscopy revealing the combination process to produce the most stable lattice, a little fine tuning would make this process the most realistic technique yet for future electronic purposes.

The last analysis performed was with DSC, which monitors the thermodynamics of a system as it goes through a phase transition. It was found that this transition occurred at -24°C for pure C_{60}. With each technique the aim is to push this transition closer

to room temperature and it was found that a shift of 8-9°C towards room temperature occurs for each individual technique. This indicates increased thermal stability for each technique, the greatest shift occuring for the combination process.

Overall, dramatic differences occurred for each technique. The combination process proved to be the most successful technique. Absorption analysis revealed the HOMO-LUMO to remain unchanged while there was a loss of oscillator strength at 450nm indicating a change in the packing of the molecules in the lattice. Raman spectroscopy revealed a shift of the 1469cm^{-1} mode characteristic of pure C_{60} to 1464cm^{-1} and this new feature was stable to prolonged illumination. DSC analysis showed a shift of 9°C towards room temperature, indicating increased thermal stability and with microscopic analysis revealing that the film partially retains its surface integrity it was concluded that the combination process is the most realistic method to use for future electronic purposes.

Simulations of Bound Electronic Wavefunctions within Potential Wells

David Fitzpatrick
Supervised by Dr John Doran

Personal Details

In the first two years of my BSc I studied physics, chemistry, ancillary maths, management studies and French. In third year and fourth year I replaced chemistry with Physics Technology. I enjoyed the continuous assessment of the first two years and I would prefer continuous assessment rather than just end of year exams. It made me study a lot more. I much preferred fourth year experimental labs because I could do them on my own so I learned a lot more. I enjoyed the material especially the mathematical subjects.

During the weekend I work in a Texaco garage as a cashier. My hobbies include socialising, listening to music and playing chess.

Project Summary

My final year project involved the simulation of a potential well. This potential well confines an electron inside it. The electron is bound by the well's potential and because of this it is confined in discrete energy levels in the well.

This physical situation occurs in a number of real life applications. One such example would be the confinement of an electron in a metal sheet. The electron is free to move perpendicular to the sheets surface but it must overcome a certain potential to free itself from the metal. The potential in this case is the work function of the metal.

Quantum Mechanics states that light and matter exhibit wave-like as well as particle-like behaviour. Therefore an electron is both a wave and a particle. In this project it is treated as a wave. Its motion is described by its wavefunction Ψ.

The probability density is the modulus of the wavefunction squared. This is the probability of finding the electron in a certain region. It therefore ranges from zero to one.

In the *finite* potential well the electron is confined in certain energy levels due to the well's potential, Vo and width, Xo. The electron is treated as the wave in figure 1. The square of the wavefunction is proportional to the probability of finding the electron in this region of the well. Since the wavefunction crosses the well edges there is a small but finite probability of finding the electron outside of the well also.

The realistic energy levels of the electron in the well are those levels that do not diverge to infinity too soon at the well edges. For different wells of differing potential energies Vo and differing widths Xo, there are certain fixed energy values that an electron can contain in the well. These are found by numerical approximation (using the program Matlab in this project).
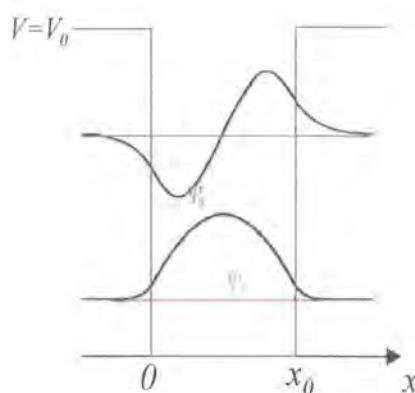
Figure 1. Finite potential well showing first (ground) and second energy states and the associated wavefunction shape for a confined electron.
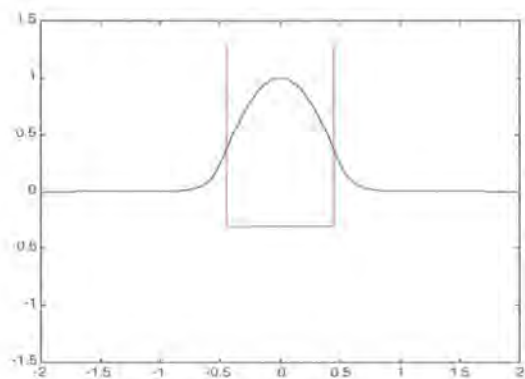
Figure 2. Calculated wavefunction of electron for first energy level in well.
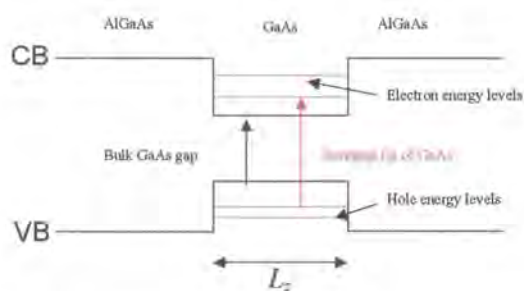
Figure 3. Schematic of a GaAs potential well sandwiched between two AlGaAs layers.

The objective of this project was to produce computer programs in Matlab that would calculate the first energy level of an electron in a particular potential well and graph its wavefunction.

Applications of this potential well include the simulation of semiconductor materials. Quantum potential wells are grown in semiconductor materials to restrict or pass electrons. They are also used to make light emitting diodes (LEDs). In the case of Figure 3 for example, a GaAs potential well was grown in between two AlGaAs layers. For differing widths Lz of the well, different energy levels of the electrons and holes occur.

When the electron moves from the CB to the VB it emits radiation proportional to the energy it loses. Differing bandgap energies produce different wavelengths of radiation. Differing wavelengths of radiation produce differing colours of light. Therefore for the LED different colours of light are emitted. So a quantum well with a well-defined bandgap will give a specific colour of light.

Cold Gas Plasma-Induced Surface Activation Effects

David Fleming
Supervised by Dr Des O'Mahony

Personal Details

Having completed the Technician Diploma in Applied Science in 1999, I decided to continue with my studies and pursue a Degree in Physics & Physics Technology. Before completing my degree, I worked in the National Metrology Laboratory for three months. I was assigned the task of developing an 'Acoustic Volumeter' to give even more accurate mass measurements than the system currently in use. I then worked for ten months as a research assistant in FOCAS, a developing research institute within DIT Kevin St., before starting my final year.

My academic interests include Nuclear Physics, Medical Imaging, Lasers and of course, Plasmas. My hobbies include blues guitar, golf and socialising.

Project Summary

Plasma is referred to as the '4th State of Matter' and is essentially a highly ionised gas. This ionisation can be provided by a number of different mechanisms. The source chosen for this project was 900V passed across two electrodes within an evacuated

Figure 1. Atmospheric plasma used in this work showing striations in this case in the presence of a magnetic field.

glass tube acting as a chamber. A Tesla coil was used to initiate the plasma and cause an electron avalanche. Once 'sparked', the plasma was quite evident and glowed a pink/purple colour – typical of an atmospheric process gas (see Figure 1).

In order to characterise the plasma, it was necessary to take a number of measurements. The variables pertinent to the discharge tube were Pressure, Voltage (and thus Current), and Time. It was found from Optical Emission Spectroscopy techniques and various tests on substrates, that the optimum requirements for activation were: Voltage $\approx$ 700V, Pressure $\approx$ 0.65mbar, Current $\approx$ 20mA. It was also found that the ideal region for activation within the chamber was directly beneath the cathode, where there was a very high density of highly energetic, heavy ions.

When a material is placed within an evacuated chamber and exposed to a plasma, the material's surface can become modified. The extent to which it is modified depends on the material, the type of plasma and the exposure time. Plasma applications include cleaning, etching and surface activation, which may disrupt or even remove the upper layer of a material essentially leaving a layer of open and highly reactive bonds. These bonds are willing to bond with any material in contact (are said to have a high surface energy) and so are ideal for the better adhesion of thin films.

By using the 'Sessile Drop' test, it was possible to see the macroscopic effects of plasma on a material i.e. a surface's wettability increased on plasma exposure (Figure 2). The proof of this was through the drop test. A material that was hydrophobic (low

Figure 2. The sessile drop test involves placing a small volume drop onto a material and measuring the contact angle between drop and surface.

surface energy) meant that water beaded up on it – they practically repelled each other and the main force keeping them together was gravity. The same material, after approximately 2 minutes' plasma exposure became hydrophilic (high surface energy). This meant that it was more attracted to the delicately dispensed 10µl water drop, and so the water spread outwards.

Glass reacted quite well in the plasma but, prior to plasma treatment, it was not hydrophobic enough to warrant contact angle measurements to be made. Instead, a polymer, Polypropylene (PP), was chosen to illustrate this effect. PP exhibited tremendous hydrophobicity pre-treatment, and linearly less so after approximately 1 minute of plasma treatment. Its contact angle in sessile drop tests before was 90°, and after 1 minute of treatment this reduced to 66°. After 10 minutes, the measurement was less than 30° (Figure 3).

From these contact angle measurements and from Young's Equation relating interfacial energies, the
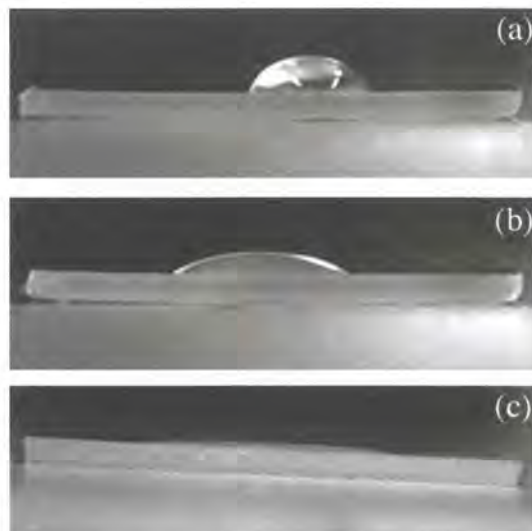
Figure 3. Drop tests for polypropelene (a) prior to plasma exposure (b) after 1 minute of exposure and (c) after 10 minutes of exposure. The same volume drop is used in each case and the variation of contact angle is clear.

Spreading Function of Polypropylene was found.

Due to time constraints, thin film deposition on activated surfaces could not be analysed. However, an atmospheric process gas was analysed thoroughly for plasma modification and a technique of contact angle analysis for examining the surface tension of a material after plasma treatment was incorporated and proved to be a quite successful one.

Hopefully, my project report may help future final year students who choose to undertake similar investigations.

Determination of the UV-VIS Transmission of Contact Lenses

Chanel Hayden
Supervised by Dr James Walsh & Linda Moore

Personal Details

After completing my Diploma in Applied Science, I spent almost a year travelling in Australia, New Zealand and Asia where I learned to surf, scuba-dive and ski. Upon my return I immediately began a follow-on degree course in Physics and Physics Technology.

Last summer, I was employed as a Research Assistant by the Facility for Optical Characterisation and Spectroscopy (FOCAS) at DIT Kevin St. where I gained valuable experience in the spectroscopy field. I put this experience to good use on my final year project, which is summarised below.

Project Summary

Ultraviolet radiation is made up of 3 bands: UVA, UVB and UVC. UVB is the biologically active part of the spectrum that causes skin cancer and ocular damage. Eye diseases such as cataracts and snow-blindness have been attributed to extended exposure to UV radiation. Since depletion of the Ozone layer began, the amount of UV radiation reaching the Earth's surface has increased by 3% over the last decade. This has prompted some contact lens manufacturers to add UV absorbing properties to their lenses.

Thus the aim of this project was to investigate how much UV light was transmitted by these lenses.

Two different types of spectrometers were used to measure the amount of transmission in the lenses. But first, a novel spectral transmission measurement cell was designed, constructed and tested for use with both spectrometer systems. The cell was designed to approximate as closely as possible true *in vivo* conditions.

The first spectrometer used to investigate the lenses was the LAMBDA900 UV-VIS which resides in Lab 305, one of the FOCAS facilities. Spectra of the lenses recorded with this system were compared with previous studies and then with the Ocean Optics S2000 fibre optic spectrometer.

After finding that the resultant curves compared well, the optical properties of the lenses were then examined. These studies were carried out solely with the S2000 system as it has a spot beam that can be used to target specific areas of the lens.

Optical properties such as spectral absorption coefficient and lens thickness were investigated. Spectra were taken directly through the centre and at the edge of the lenses.

Using Beer's Law for transmission T,

$$T = e^{-\alpha x}$$

the thickness x and the spectral absorption coefficient α were calculated in each case.

Figure 1. Novel transmission measurement cell constructed for this project
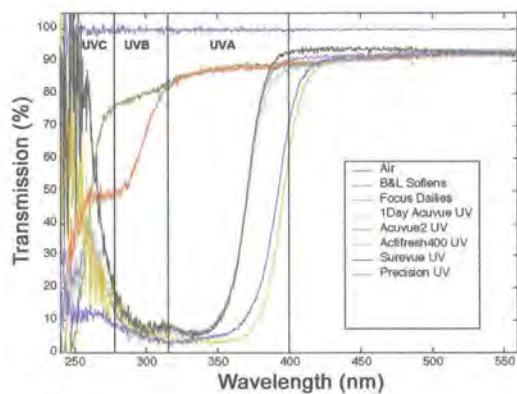
Figure 2. Transmission spectra for various contact lenses (Ocean Optics S2000 microspectrometer)
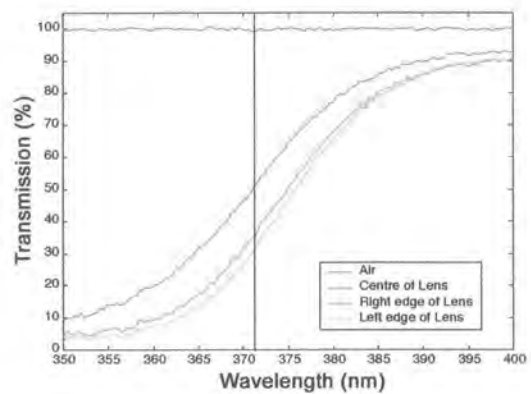
Figure 3. Surevue UV D-3.00 (Ocean Optics S2000 microspectrometer)

In Figure 2, transmission spectra for a number of different lenses are displayed. Figure 3 shows how variation in thickness across the surface of the lens affects transmission. A negative power lens was used i.e. a concave lens. This means that it is thicker at the edges than in the centre of the lens and so it transmits more light through the centre.

Quantised Conductance in Nanocontacts

Alan Kelly
Supervised by Elizabeth Gregan

Personal Details

I transferred into the third year of the BSc after already achieving a Diploma in Applied Physics and Instrumentation at the Institute of Technology, Tallaght. During that year I studied Mathematics, Physics, Physics Technology, German and Management studies. My final year subjects comprise Physics and Physics Technology. I am interested in scientific research, especially in the area of nanotechnology, communications, microwaves and all areas of Solid State Physics. My hobbies include reading, keeping fit and listening to music.

Project Summary

An increasingly large and important area of physics is concerned with the fabrication and properties of nano-scale structures, as small as a few hundred atoms across. Such structures display a host of electrical, mechanical and optical properties not seen in larger devices and for this project I was mainly concerned with nanocontacts. A nanocontact is an area between two macroscopic bodies, where the dimensions are so small that it is comparable to the mean free path of the electrons travelling through them. In a nanocontact the quantum mechanical wave character of the electrons becomes important, thus giving the possibility of observing exciting quantum phenomena like quantised conductance. Basically the theory states that as the area of the contact between the wires decreases the amount of conduction channels available to conduct electrons decreases in steps of $2e^2/h$. This results in steps in the I/V curve when measured on an oscilloscope.

Inspired by a paper by S. Carroll, an experiment on quantised conductance in nanocontacts was created. A simple op-amp circuit was used, in conjunction with a digital storage oscilloscope to observe the conductance steps. The experiment was interfaced to a computer to accumulate a histogram of the conductance values as the wires were brought into and out of contact repeatedly. The histogram showed peaks near integer multiples of $2e^2/h$. It was the aim of this project to model as closely as possible the experimental set-up of S. Carroll, which consists of two gold wires in close contact with a small V_{bias} across them. This was connected to an op-amp and in turn to a Tektronix oscilloscope, to capture the data. A program was designed in the computer software package *Labview* which was able to control and read the internal board and external instruments. This allowed the oscilloscope screen to be shown on the PC screen. These data were then saved as a datafile for later analysis. Due to the random nature of nanocontact formation between these wires it was necessary to collect a large amount of sample traces. These traces were saved as datafiles and a *Matlab* program was written to perform numerical analysis on them. The Matlab program was also used to produce a histogram of these conductance traces which showed peaks at near integer multiples of $2e^2/h$. The traces used to
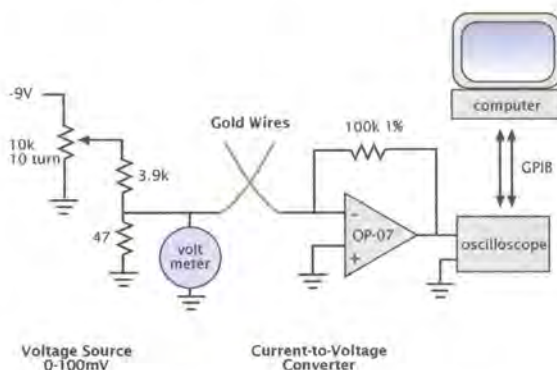
Figure 1. Experimental set-up showing the constant voltage supplies in the mV range and the I-V converter, which were contained in an aluminium box.

create this histogram were selected under strict criteria, i.e. the criteria used to define a conductance step.

The results of this project question the ease with which quantised conductance steps and hence a histogram with peaks near integer multiples of $2e^2/h$ can be achieved. It also offers valuable exposure to a current research topic in condensed-matter physics, which ordinarily is inaccessible at undergraduate level. The project provided an interesting insight into the area of nanotechnology and quantum mechanics and I would very much like to continue research in this area.

Figure 2. Experimental apparatus and worbench.

Figure 3. The LabView program.

An Investigation of the One-Dimensional Ising Model

Sa'id Koya
Supervised by Dr Des O'Mahony

Personal Details

I transferred into the third year of the BSc after already achieving a Diploma in Applied Physics and Instrumentation at the Institute of Technology, Tallaght. During that year I studied Mathematics, Physics, Physics Technology, German and Management studi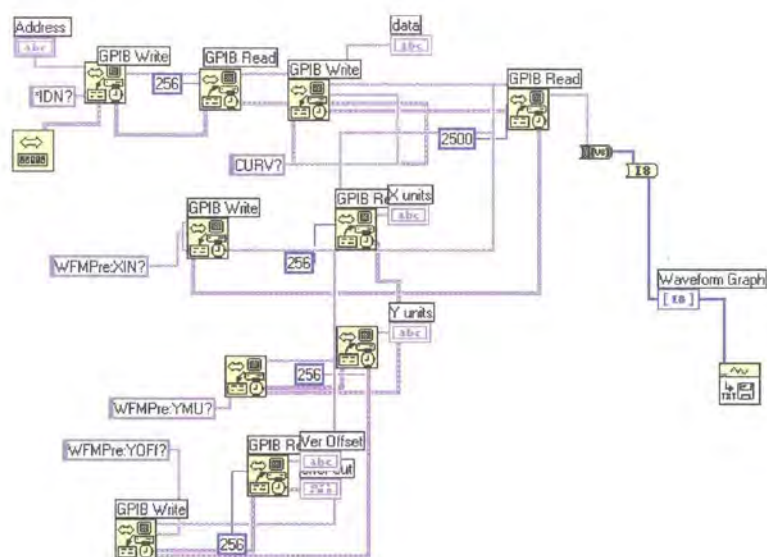es. My final year subjects comprise Physics and Physics Technology. I am interested in scientific research and developments in information technology, methods of communication, microwaves, lasers and optics. My hobbies include reading, playing and watching sport and listening to and playing music.

Project Summary

My final year project involved creating and analysing a computer-based Ising model. Initially I carried out a literature review to gather the details of the Ising model and to determine how I could create/simulate it. The Ising model is a very basic one-dimensional model of the behaviour of simple magnets and is relatively straightforward to model. I decided to use the C programming language to create an Ising model on a computer, as I had experience in using C through classes in Computational Physics.

Magnetic materials comprise of magnetic spins. In the model, the spins have a choice of either being up ($\uparrow$) or down ($\downarrow$). The model basically simulates a chain of these spins, like that shown in Figure 1. I simulated 200 spins in the model, to get a good statistical set of results from it. Two types of magnetic materials can be simulated in this model, a ferromagnet and an anti-ferromagnet. A ferromagnet is a material that is magnetic to start with. It has more spins aligned in one direction than another, (i.e. most of the spins pointing up) which causes it to be magnetic. An anti-ferromagnet is a material that starts off demagnetised, with an equal amount of spins in each direction, but becomes a very strong magnet if an magnetic field is applied.

During my research, I found a step-by-step set of rules, which I used to write my program. It is called the *Metropolis Algorithm*. This governs the orientation of the spins, using equations for the energy of a chain of spins and probability. It also makes use of random numbers.

This led to the question: can a computer give a *true* random number? I discovered that in reality a computer uses a deterministic method for generating random numbers, therefore they cannot be truly random. However, for the purposes of experiments here, they can be considered as random because if you were to look at them you would not see any obvious connection between the numbers. This is called pseudo randomness. I found a pseudo random number generator, written in C, and adjusted it for use in the Metropolis algorithm.

Finally, using two equations researched earlier, I included in the program a function to calculate the magnetisation of the material being studied and a
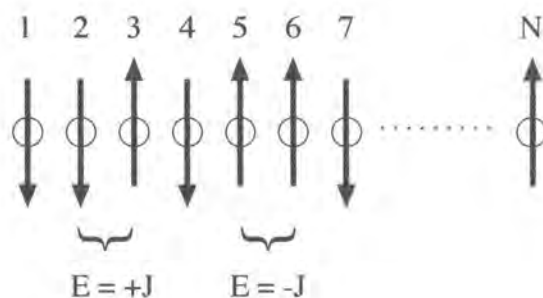

Figure 1. Chain of N magnetic spins showing the interaction energies +J and -J that are possible for each pair.
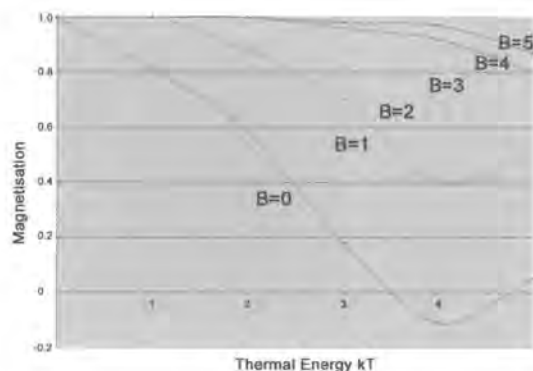
Figure 2. Graph of magnetisation as a function of temperature for a 1D ferromagnet model.

function to calculate the total internal energy of the material. I then set input parameters of thermal energy and applied magnetic field, to allow the study of the behaviour of the spins/material when these were changed. I recorded the magnetisation and internal energy for a series of thermal energy and magnetic field values, for both the ferromagnetic and anti-ferromagnetic materials.

Figure 2 is a graph of magnetisation for a ferromagnet showing that the magnetisation drops as thermal energy increases, and that the application of the magnetic field makes it harder for demagnetisation to occur because of thermal energy.

There are still a few things that could be done to advance this experiment. I studied only a one-dimensional model, while two- and three-dimensional models can be created. There are also a few other properties that can be studied for the one-dimensional model, such as calculating the specific heat capacity of the material. Overall I enjoyed working on this project and would like to continue to study and research this topic.

Spectroscopic Study of the Manufacturing Process of Contact Lenses

Sharon McDermott
Supervised by Dr Robert Howard

Personal Details

I started my academic career in the Institute of Technology Tallaght in 1997, where I obtained my Diploma in Applied Physics & Instrumentation, with grade Merit 1. In 2000 I transferred to DIT Kevin Street to undertake a BSc in Physics & Physics Technology. During the summer of 2001 I was employed as an Analytical Technician in the spectroscopy department in Hewlett Packard. While working there I gained a lot of practical experience and a keen interest in spectroscopy. I am very interested in travelling and have travelled extensively through Europe. In the near future I am hoping to travel around the world. My hobbies include reading, amateur dramatics and socialising.

Project Summary

Most contact lens manufacturers use ultraviolet (UV) fluorescent lamps in the manufacturing process to initiate photopolymerisation. Photopolymerisation is the use of light to initiate a polymerisation reaction, i.e. convert a liquid monomer to a solid polymer by means of a chemical reaction. However, there are a number of disadvantages in using these lamps. The intensity of the UV radiation being emitted is very important to ensure the quality and reliability of the lenses but since the intensity of these lamps decrease over time they have to be constantly monitored and replaced frequently. The other disadvantage in using these lamps is that they must be activated at least fifteen minutes before they can be used in the photopolymerisation process; this is to ensure that the lamps have sufficiently warmed up.

The aim of this project was to see if it is possible to replace these lamps with an alternative UV light source, a UV light emitting diode (LED). It is expected that these sources will be more stable and their intensity will be constant over time. If it is possible to replace these lamps it will lead to reduced costs and down-time for the manufacturers.

Photopolymerisation is achieved by adding a light-sensitive compound to an appropriate polymerisable substance; the light-sensitive compound is then activated by light of an appropriate wavelength and converts the absorbed light energy into ions or free radicals. The type of light-sensitive compound used in this project was a photoinitiator, called 2,2-dimethoxy-1,2-diphenylethan-1-one, which is more commonly known as Irgaure 651. The photo-initiator initiates photopolymerisation and the curing process in the monomer mix. Irgaure 651 is UV active. The polymerisable monomer used in this project was 2-hydroxyethyl metacrylate (HEMA). HEMA is a hydrogel-based material, which can be made into soft contact lenses.

A small drop of the solution was placed on to a glass slide and the UV light source was placed directly above it. The glass slide and the light were placed into a resealable bag and flushed with nitrogen gas in order to exclude any oxygen, which would have inhibited polymerisation. The light source was then switched on and the solution was allowed to polymerise for a period of time. Both the Raman and the Fourier Transform Infrared (FTIR) spectrometers were used to monitor the polymerisation process. The spectra obtained by both techniques were very similar in information. As both techniques will complement each other they will help to fully characterise the polymerisation process.

The vibrations used to monitor the curing process were the C=O bond at $1718cm^{-1}$, C=C bond at $1636cm^{-1}$ and the C-O-C bond at $1174cm^{-1}$. The C=C bond is directly involved in polymerisation and as a result it should get used up and fully disap-
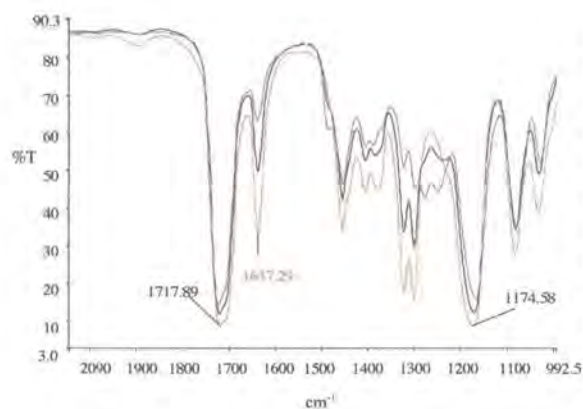
Figure 1. FTIR spectra recording the curing process of HEMA over 70 minutes

pear if polymersiation has occurred. The C=O and the C-O-C vibrations are used as references and should not change during curing. The progressive decay of the C=C band over time was observed both in the Raman and in the FTIR spectra. The degree of curing was determined by comparing the peak height of the C=C band to the peak height of the reference bands.

Polymerisation of HEMA was observed in both the Raman and the FTIR spectra during this project, from this it was concluded that the alternative UV light source did initiate photopolymerisation in the monomer mix. This proves that this light source has the potential to replace the UV fluorescent lamps that are currently being used in industry.

Plasma Activation of Biomedical Polymers

Andrew Norris
Supervised by Dr Denis Dowling & Dr Miriam McConnell
(Enterprise Ireland) and Dr Des O'Mahony (DIT)

Personal Details

In the first two years of my BSc I studied physics, chemistry, ancillary maths, management studies and German. In third and fourth year I replaced chemistry with physics technology. I have worked in the National Metrology Laboratories (NML), and conducted this project in Enterprise Ireland's Surface Engineering Department. My hobbies include reading, playing and watching sport and listening to and playing music.

Project Summary

Biomedical polymers are simply polymers utilised in biomedical applications, that satisfy any physical requirements for their application and are biocompatible. This biocompatiblity involves them having low friction coefficient values and being hydrophilic. Since biocompatibility involves the interface between the device and its biological environment, surface modification techniques can be used to modify the surface of the polymers to make them more suitable to different environments.

This project involved using plasmas to interact with biomedical polymer surfaces, where the energetic species in the plasma change the surface structure, creating different functional groups, which modify the surface energy and hence the surface properties.

For this study, the biomedically important polymers, Polyurethane, Polyethylene, Silicone and Nylon were used. The polymers were treated in a novel 'non-equilibrium' hybrid microwave (MW) plasma generator with a wide variety of parameters being varied. These directly affect the chemical and physical characteristics of the plasma and subsequently affect the surface chemistry obtained by plasma activation. Process parameters such as gas type, (Argon and Nitrogen), treatment power, treatment time and source substrate distance were varied.

Alterations to surface specific properties upon plasma treatment, such as topography, friction coefficient values and surface wettability were determined using optical microscopy and atomic force microscopy (AFM), a Pin-on-Disk friction measurement unit (Tribometer), and an FTÅ200 Contact Angle Measurement Unit respectively.

The 'non-equilibrium' plasma generator used in this project allows the heavy species to remain at low temperatures and is exactly what makes the plasma useful, allowing high-energy chemistry at low physical temperature. A microwave plasma generator was employed as it is found to be more efficient at producing active species than its counterparts, such as the RF systems and DC systems.
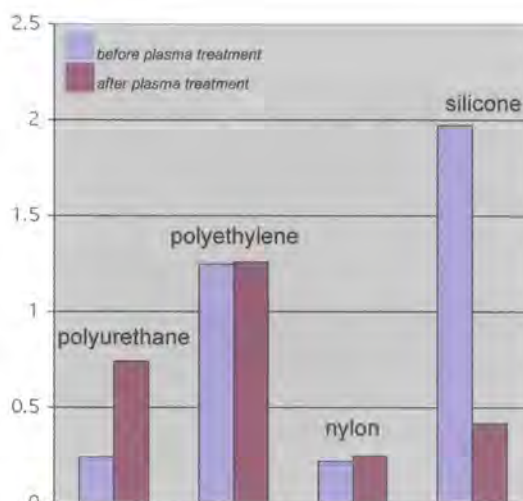

Figure 1. Friction Coefficients after 500 pin-on-disk revolutions with a load of 10g applied.

The various polymer surface properties were determined prior to activation and afterwards to enable determination of the effects of the plasma activation. Following treatment, optical and atomic force microscopy essentially showed little or no alteration of surface morphology. This ruled out the occurrance of plasma processes such as etching deposition and damage.

Using pin-on-disk measurements with 500 revolutions and a load of 10g applied, increases in μ values were observed in all cases except Silicone, with Polyurethane showing the greatest increase. Decreasing the source substrate distance also increased the value of μ obtained, as did increasing the treatment time. These varying effects are a result of different levels of oxygen incorporation.

The contact angle (measure of wettability) results, detectable by eye, also showed clear effects and it was deduced that this was due to oxygen incorporation which resulted in surface bonds becoming increasingly polar.

In conclusion, polar bond formation due to oxygen incorporation as a result of the plasma treatment strongly influences biomedically important surface properties.
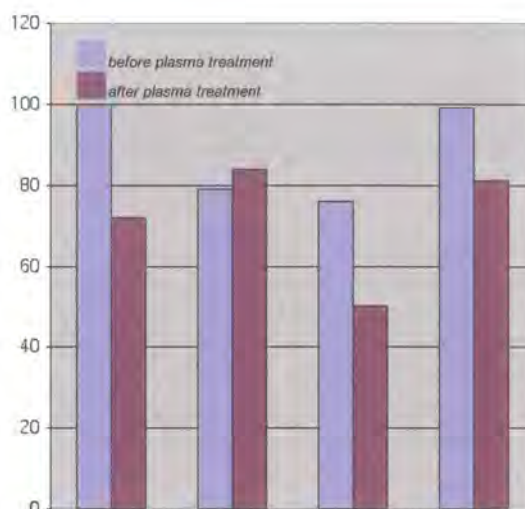
Figure 2. Contact angle measurements before and after plasma treatment for (left to right) polyurethane, polyethylene, nylon and silicone.

Construction and Characterisation of an Organic Molecular Field Effect Transistor

Barry O'Connell
Supervised by Dr Hugh Byrne & Dr Gordon Chambers

Personal Details

A graduate with a Diploma in Applied Science, I specialised in the Applied Physics option before transferring into the BSc Physics and Physics Technology course in DIT. I have 15 months full-time work experience in the DIT working for the POMM (Physics Of Molecular Materials) group and FOCAS (Facility for Optical Characterisation And Spectroscopy). During my work in these groups, I gained practical knowledge in many fields including Spectroscopy, Instrumentation and System Administration. During this period of employment I wrote the software to control and assisted in the construction of an Electroabsorption Spectrometer. My personal interests include multimedia and modern music composition and I host a radio show once a week.

Project Summary

My final year project involved the design and construction of a Thin Film Organic Molecular Field Effect Transistor using carbon$_{60}$ (C_{60}) as a transport layer. The main objective was to produce and characterise a reliable and easily reproducible device, which could be used in conjunction with existing equipment.

Carbon$_{60}$ is a large spherical molecule made from 60 carbon atoms that was discovered in 1985. It is structurally very stable and each of the atoms contributes a single delocalised electron to the molecule. It is these 60 delocalised electrons and what they do that makes C_{60} a very interesting subject to study. Under certain conditions, C_{60} has been seen to switch between metallic, non-conducting and even superconducting states. Characterising similar behaviour changes wasthe underlying motivation for this project.

The first problem was to create a design which would allow the device to be constructed using only thin films. The device was constructed as shown in Figure 1. The gate electrode was the first layer to be deposited, followed by the oxide layer, which was around 80nm thick. Then the source and drain electrodes were evaporated, these were separated by a gap of 40 microns, and it is into this gap the C_{60} goes. The depth of this gap ranged from 120nm to 250nm. Glass slides were used as masks to prevent the layers interfering with each other during evaporation. The 40 micron gap was made by taping a Mylar fibre across the device as a mask before the source and drain electrodes were evaporated. The oxide layer prevented current flowing from the gate but it would allow an electric field to affect the current flowing through the C_{60}. A photograph of the first working device produced is shown in Figure 2.
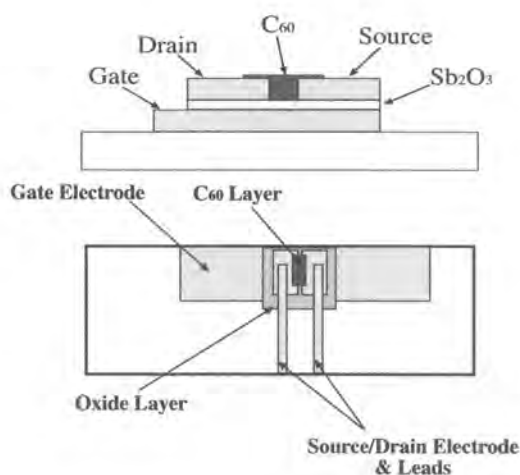
The behaviour of the device was then examined.

Figure 1. Schematic of device construction.

Figure 2. Working device based on the schematic of figure 1.

The current flowing between the source and drain electrodes was measured for a series of voltages whist different gate voltages were applied. This revealed some very interesting behaviour as seen in Figure 3. Some of these results have already been seen in a similar device that consists of C_{60} sandwiched between two electrodes, currently under study by the POMM group. The device also showed a lattice reorganisation due to charge present in the device and a corresponding shift in the device's resistance.

Three working devices were made, demonstrating that the design is a practical one. The project concluded with an attempt to reduce the size of the device to fit it into a cryostat. This would allow the device to be brought to a low temperature whilst simultaneously allowing in-situ electrical measurements and reflection spectroscopy. The reason for this is to further the study of the mechanisms associated with the device's behaviour, which are not fully understood. The device in its current incarnation has much more work to be done on it regarding characterisation. This project has greatly enhanced my work experience and is an area in which I hope to continue working. Some of the results of this project have been published in the proceeds of the MRS Spring meeting 2002, see S.B.Phelan, B.S.O'Connell, G.Farrell, G.Chambers & H.J.Byrne, MRS Spring Meeting, San Francisco (April 2002).
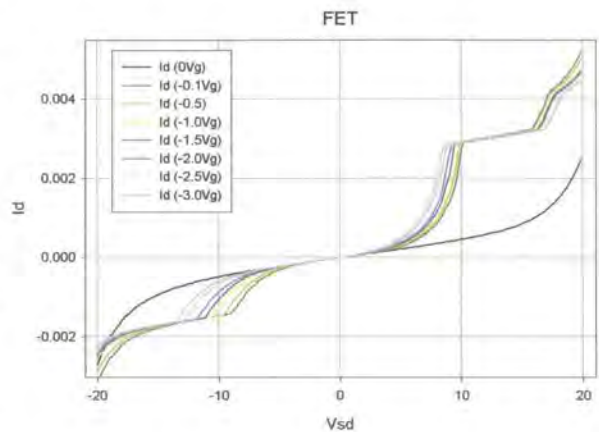

Figure 2. Source-Drain current as a function of voltage for set gate voltages

Carbon Nanotubes for Molecular Recognition

Luke O'Neill
Supervised by Dr Hugh Byrne & Elizabeth Gregan

Personal Details

My first three years in DIT Kevin Street were spent on the Diploma course in Applied Physics; from there I went on to study the BSc in Physics and Physics Technology. Over the past years in college I have maintained different part-time jobs as well as pursuing my interests in reading and writing. I have represented my county at athletics and am also an avid soccer and gaelic player. I have other hobbies including socialising and collecting comics and books.

Project Summary

Last year research was carried out using the organic polymer PmPV to solubilise and purify Single Wall Carbon Nanotubes (SWNT). It was chosen as its chemical structure allows the coiling of the backbone around the tubes. Furthermore, the presence of floppy sidechains allows the suspension of nanotubes in solution. When the tubes were introduced into the PmPV solution, the fluorescence of the solution increased significantly and this increase could not be accounted for by any slight change in concentration. This indicated that the nanotubes were acting as nano-spacers, preventing the polymer from aggregating.

This project branched out from the study undertaken last year and involved using raw nanotube soot and two simple dye molecules, anthracene and terphenyl, in various solvent solutions. The reasoning was that if the molecules were small and of the same order of magnitude as the nanotube lattice it would be possible to get molecular mapping as shown in Figure 1.

Terphenyl consists of three-fused phenyl rings but these are coupled via a single carbon bond. Figure 1 shows the suggested interaction that this project was designed to investigate. It was essentially a step back from the complex organic polymer used previously to a simple organic dye that could map

directly onto the surface of a Zig-Zag tube and therefore isolate the individual tube.

The aim of this project was to investigate the interaction outlined in Figure 1. Various analysis techniques were used to explore this interaction and elucidate the dye molecule interaction with the SWNT. Fluorescence and UV/Vis/NIR spectroscopy were employed first to determine if there is any interaction between the tubes and the dye. Spectra were obtained for the different dyes on their own at varying concentrations. Then a concentration was selected and the tubes were introduced into the solution. A spectrum of the tubes and dye (hybrid) solution was then taken. The hybrid spectrum and the original spectrum were compared and as there were changes in fluorescence which were not concentration related then it was assumed that interaction had occurred.
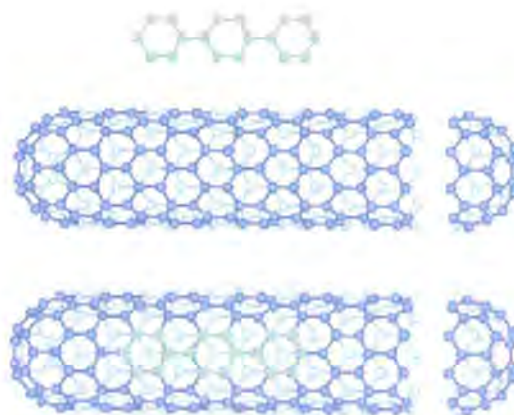

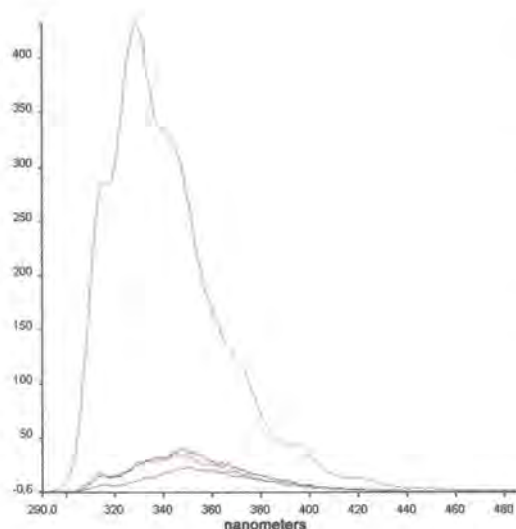Figure 1. Proposed mapping of terphenyl to carbon nanotube

Figure 2. Fluoresecence spectra of terphenyl with and without (pink plot) tubes

Further investigation was undertaken using Raman spectroscopy. This provided information both on the dye, raw tube and the hybrid, as they all have distinct spectral features. As the Raman spectrum of the hybrid is not a superposition of the raw dye and the raw tube, then this confirms that an interaction has indeed taken place (Figure 3).

These techniques provide information on the nature and extent of the interaction taking place between the dye and the tubes. This information will hopefully lead to the solving of the problem of nanotube processing. The aim of this project was to observe and try to quantify the interaction of a simple dye molecule, terphenyl, with SWNT. The first major improvement that was noticed was that with the dye in solvent the tubes were held in solution. This was a major sign of interaction as without the dye the amount of SWNT that stayed in solution was negligible. The next evidence of interaction was the fluorescence quenching observed when the tubes were introducing into the dye toluene solution (Figure 2).

From Raman spectroscopy it was seen that the raw terphenyl and the raw SWNT had a peak overlap which would allow for vibrational coupling and therefore a transfer of energy. Raman also shows that the G-Line and RBM line were present in the interaction spectrum indicating the presence of the tubes (Figure 3). Raman spectrum of the hybrid is more than the sum of the individual components, showing new peaks signifying interaction.

In summary the non-destructive effects of the terphenyl molecule on the SWNT are:
• It functionalised the tubes allowing them to be dissolved in the toluene solution
• Fluorescence quenching indicated energy being coupled to tube lattice and also indicated that the molecule is mapping straight on to tube.
• Further evidence for vibrational coupling was provided by Raman spectroscopy where it was seen that terphenyl and tubes had over-lapping peaks.
• Raman also showed a tube/terphenyl interaction containing peaks that were not characteristic of either the tubes or terphenyl.

The results were included in "The use of Single wall Carbon Nanotubes as templates for organic molecules", T.G. Hedderman, L. O'Neill, S.M. Keogh, E. Gregan, B. McCarthy, A.B. Dalton, G. Chambers, H.J. Byrne, to be published in Proceedings of International Winterschool on Electronic Properties of Novel Materials, Kirchberg, Austria, March 2002.

Figure 3. Raman Spectra of tubes, terphenyl tube mixture and raw terphenyl

Investigation of the Vibrations of a Thin Steel Plate

Séverine Philippe
Supervised by Patrick Healy

Personal Details

I first completed a technician diploma on physical measurements, instrumentation and process control in Université de Savoie (France). After that, I worked six months on the process of preparation and dispersion of mineral additives in polymers for the firm Coatex (France). I then left for Ireland and entered the final year of a Diploma in Applied Sciences - Physics Option at the DIT, and was awarded a Distinction. I worked for Daewoo (France) in a cathode ray tube factory as a technician of the Quality Department, before completing my degree in Physics and Physics Technology. My hobbies include playing and listening to music, hiking, swimming and practising martial arts.

Project Summary

The object of my project was to investigate the vibrations of steel plates using the ANSYS computer package to find the different mode frequencies and observe their shapes. Then I tried to verify some of these results by performing two different experiments. The first experiment aims at finding the vibration frequency spectrum of a square plate and the second one aims at observing sand patterns showing nodal shapes.

The analytical solution of the vibrations of a solid elastic plate came quite late, though E.F.F Chaldni obtained much experimental information in the latter part of the 18th century. In 1787, he described his method of using sand sprinkled on vibrating plates to show the nodal lines. The exact forms of his figures defied analysis for many years and it was Sophie Germain who gave the correct fourth order differential equation in 1815. Her choice of boundary conditions proved, however, to be incorrect. It was not until 1850 that Kirchoff gave a more accurate theory. The problem still provides considerable interest for scientists even at the present time, both along theoretical and experimental lines.
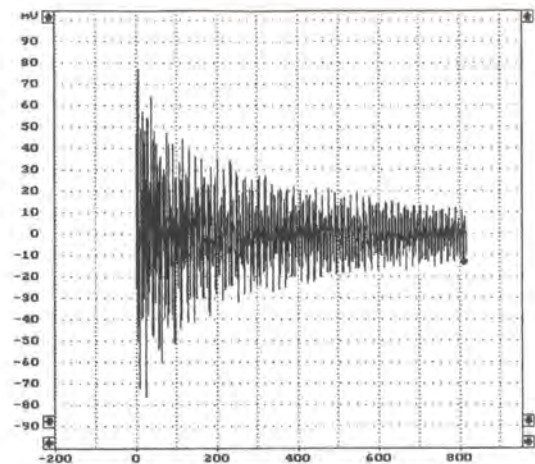

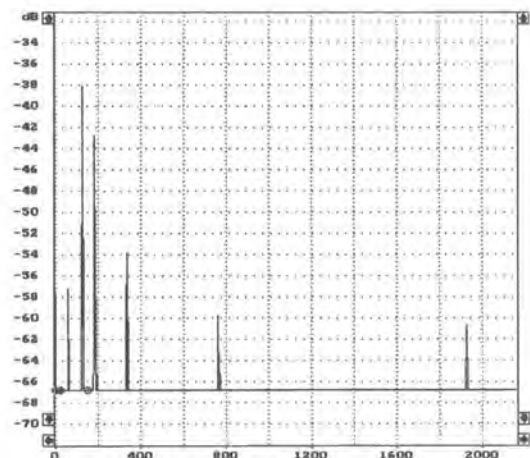*Figure 1. Time spectrum of accelerometer output obtained from striking the plate*

Figure 2. Frequency spectrum of accelerometer output derived from Figure 1

During this project, a modal analysis was performed using the ANSYS finite element analysis package. First a geometric model of a steel plate was built. It was then meshed into a finite element model. Finally the boundary conditions were defined by applying constraints to some of the nodes. From there the different modes of vibration of the plate could be expanded and visualised.

It was then decided to try to verify some of these results using a real steel plate and an accelerometer. The plate was impacted and the output of the accelerometer (Figure 1) was analysed using Fourier analysis (Figure 2) to see if the modal frequencies found with ANSYS were the same as those found on the frequency spectrum of the vibrating plate. Some differences were found: some of the modal frequencies were not present in the spectrum and those present tended to be slightly higher than expected. This was mainly due to defects in the symmetry of the plate and dislocations present in the material.

Another way of exciting the plate was to use a bow to select only one mode at a time. The modal patterns were visualised by sprinkling some sand on the plate. When the plate vibrates, the sand gathers at the nodes of the vibration. Only four different modes could be excited due to the thickness of the plate (2 mm) but also due to the fact that in order to be excited by a bow, these modes must have antinodes on the edge of the plate. The frequencies at which we obtained these modes were higher than expected, mainly because, when bowed, the plate was not strictly speaking free at the edges. One of the sand patterns and its corresponding ANSYS simulation are given in Figures 3 and 4.

Further experimental work could involve driving the plate at given frequencies using a coil (and a magnet if necessary). The mass of the accelerometer should also be reduced. Vibrational holography could also be used (then no accelerometer would be needed) but it involves much more equipment and cost.
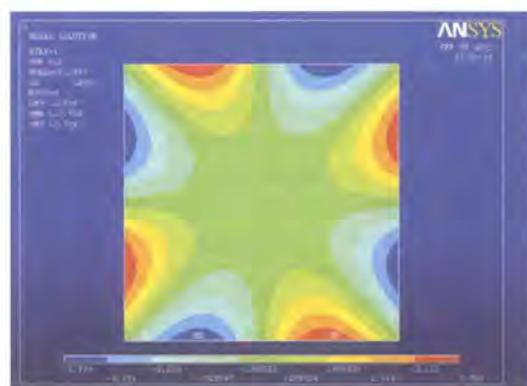

Figure 3. Mode of frequency 554Hz - ANSYS simulation.

Figure 4. Mode of frequency 643Hz - bow experiment.

Computerised Technique to Determine and Analyse the Coefficient of Restitution

Paul Ryan
Supervised by Dr Breandán Ó hAnnaidh

Personal Details

I began my study of Applied Science in September 1998. During the first two years of my degree I studied a blend of core science subjects, Physics, Chemistry and Mathematics combined with Management Studies and German. In third and fourth year my chosen option subject, Physics Technology, substituted Chemistry. Combining a study of practical physics technologies with theory based physics has been both a beneficial and a thoroughly enjoyable experience.

I have a diverse range of scientific interests including Medical and Biophysics, Optical Communications and Nuclear Physics. Another associated interest is the application of computers in science and education generally. My hobbies include Photography, Music and work with the Society of St. Vincent de Paul.

Project Summary

The aim of the project was to develop a PC based method to record the sound produced by a ball bouncing on a rigid surface and then to analyse these recordings to determine the coefficient of restitution.

Defined by Newton (c.1680), the coefficient of restitution has been the subject of numerous research papers over the years. In particular, mechanical systems to determine the coefficient have been in a constant flux of development since the early seventies. Indeed the scientific journal *American Journal of Physics* has had on an intermittent basis papers devoted to research on this topic.

The word 'restitution' in the Oxford English dictionary is defined as "*a return to or restoration of a previous state or position*". This describes the physics involved in the coefficient of restitution. The coefficient of restitution may be related to the ratio between decreasing heights. Figure 1 below illustrates the decreasing height of a bouncing ball.

Recalling childhood experiences of playing with bouncing balls it is easy to correlate experience with the behaviour shown in Figure 1. Essentially the coefficient of restitution, denoted by the letter epsilon ε, for this situation may be described by Equation (1) below:

$$\varepsilon = \sqrt{\frac{h_1}{h_0}}$$

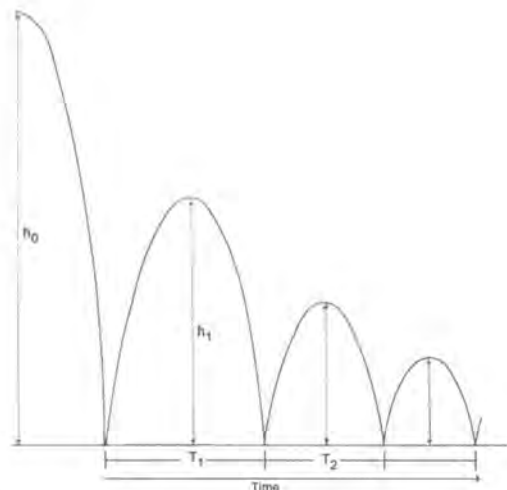(where h_0 represents the initial height and h_1 represents the 1st rebound height).

Figure 1. Schematic representation of the bounces of a ball spread out over time.

Using simple mathematical relationships it is possible to describe the coefficient of restitution both in terms of velocity before and after an interaction and the time between bounces. Equation (2) below illustrates the more useful form of these expressions, the time relationship:

$$\varepsilon = \frac{T_2}{T_1}$$

(where T_1 represents the time taken for the first bounce, T_2 represents the time taken for the second bounce).

It is clear that the coefficient of restitution is basically an expression of how well the ball will bounce. Essentially describing the elasticity of a ball, the coefficient has a value between 0 and 1 where a ball possessing a high coefficient of restitution is termed a happy ball.

The sound pattern produced by a bouncing ball is illustrated in Figure 2 below. In this picture one may see the peaks created by the impact of the ball with the surface.

Using *MatLab* I wrote a program to analyse sound patterns similar to Figure 2. Affectionately called CORA – *Coefficient of Restitution Ana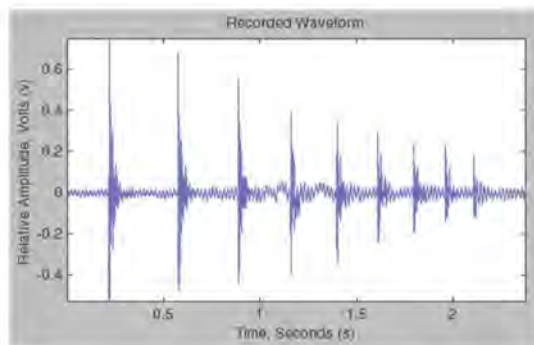lysis*, this program determined the time gaps between successive peaks and hence calculated the coefficient of restitution associated with each bounce.

The experimental procedure consisted of allowing a ball to fall from a fixed height (and thus a fixed impact velocity) onto a large slab of polished granite. This procedure was undertaken for ball specimens of various materials and for various impact velocities. Particular emphasis was placed on steel ball bearings, mainly due to their availability. An interesting observation, verified by my experimental work, was made by much of the past research. All pointed to a decrease in the coefficient of restitution with increased impact velocity. Essentially this means that more energy will be lost by a ball travelling at a high velocity when it hits off a surface than a ball travelling at low speed. Figure 3 illustrates this velocity dependence and was obtained for a steel ball bearing.

The coefficient of restitution is relevant in many areas of modern living from the obvious applications in sporting equipment such as *sliotars* (hurling balls) and running shoes to more abstract uses in the design of high performance tyres for all types of vehicles.
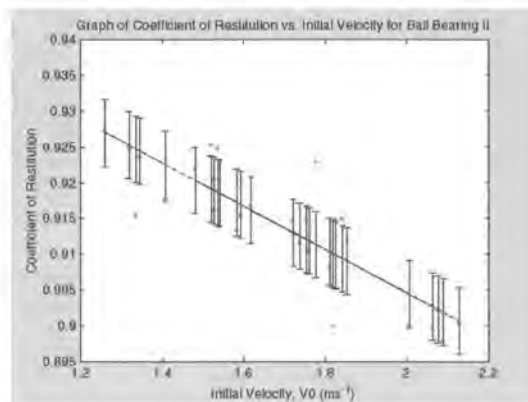

Figure 2. Illustration of sound pattern produced by a bouncing ball.

Figure 3. Coefficient of restitution dependence on impact velocity.

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