

1. Summary of the Proposed Research

Abstract:

The IRC will provide an underpinning interdisciplinary activity in Nanotechnology with the theme of accurately controlling the physical properties of nanostructures and devices by fabrication at single molecule precision. It will develop research themes and strategies that uniquely combine expertise from currently disparate fields. The primary aim is to establish the IRC as an Internationally leading centre for Nanotechnology with objectives of:

- Fabrication of complex 3 dimensional structures with molecular precision
- Growth of soft layers by directed self-assembly on patterned substrates
- Determining mechanical and electronic properties of nanoscale interfaces
- Evolving architectures for devices in biomedicine and information technology
- Spinning out several projects into the commercial sector.
- Training of personnel in interdisciplinary research.

Lay Summary:

Nanotechnology involves the manipulation and manufacture of objects on an atomic scale. One nanometer is roughly the length of three atoms in a row, or 1/10,000th of the diameter of a human hair.

We are on the brink of being able to exploit this new technology. The enormous advances made in this technology during the last twenty years mean that the tools to make and measure infinitesimally small objects have become commonplace. We will now begin to see extraordinary advances in manufacturing using these tools: computers will shrink, medical diagnosis and treatment will be almost instantaneous and non-invasive, energy wastage will be dramatically reduced and our environment will become increasingly clean.

The UK must maintain a leading role in defining this new technology, which can only be achieved by significant research and development investments. The aim of the Interdisciplinary Research Collaboration (IRC) between the University of Cambridge, University College London and the University of Bristol is to ensure that the fundamental concepts underpinning nanotechnology are fully understood. Each institution brings expertise to the collaboration:

- The University of Cambridge has expertise in nanofabrication, and the fundamentals of physics, chemistry and materials science required to fully define the properties of nanoscale materials;
- University College London has expertise in the computer modelling of such materials combined with an understanding of their theoretical physics and a background in medical applications;
- The University of Bristol has expertise in biological materials at a molecular level.

By bringing together material scientists, physicists, chemists, engineers, biologists and medical researchers in a six-year programme, we will provide a platform from which commercial exploitation will stem. By focusing the research into controlling the physical properties at the molecular scale, our work will have enormous impact; whether in developing new computer chips, medical sensors, treatments, drugs or efficient energy sources.

Building on each institution's extensive facilities, the IRC will establish centres designed for multidisciplinary research. To ensure the highest quality research and successful commercial exploitation, a Science Council and an Industrial Advisory Council will be established to guide the IRC in its venture.

Beyond the primary research role, the IRC is committed to educating researchers in nanotechnology, communicating our research widely and ensuring that we respond to public interest. We will be aided in these important responsibilities by the Institute of Nanotechnology, the leading international institution for disseminating nanotechnology to scientists, industrialists and the general public.

2. Research Objectives

The extraordinarily high level of current international funding in Nanotechnology underlines its perceived importance in forming the basis for a whole range of technologies in the next 20 years. At one extreme the precision required to fabricate ever-faster more compact computers will rely on fabrication methods with sub-nanometre precision. At the other extreme completely new types of devices are expected which will revolutionise health care and quality of life. This technological breadth arises from the fact that nanotechnology represents a physical dimension to which all the conventional science and engineering disciplines are converging. This convergence makes necessary the establishment of interdisciplinary research for exploitation from which new technology will evolve.

In establishing an IRC in Nanotechnology a priority is to position the objectives and mission of the IRC within the much broader interpretation of nanotechnology. To prevent dilution this inevitably involves clear focussing of the IRC. To be effective and credible this means a contribution at a fundamental level, from which firmly based science and technology can emerge (given the fundamental nature of the research, it is hard to predict where results will impact on technology, so that a very flexible structure for technology transfer is required).

At the base of this programme, and indeed any exploitation of nanotechnology, is the requirement to grow and to control with single molecule precision. This is the **core mission** for the IRC.

Intensive activity across all branches of science and engineering will play a major role that the IRC will realise by combining key scientific skills with a commitment to an inter-disciplinary approach. The big prizes— of ideas, techniques and ultimately new devices – present a significant challenge in the Universities to find the right structure to facilitate the requisite cross-disciplinary activity.

The IRC proposed here is directed at the very core of nanotechnology and as such will aim to provide an underpinning interdisciplinary activity with the general theme of fabrication and organisation of molecular structures. Central to the ethos of the IRC will be the development of research themes and strategies that combine expertise from currently disparate fields. The consortium will develop the basic tools to organise molecules at the hard/soft interface (the growth of ‘soft’ molecular structures off ‘hard’ substrates) by natural and other means, including self-assembly and soft lithography. Characterisation of structural properties of the interface and their inter-relationship with electronic properties is also central, and an appropriate range of tools will be available. This includes scanning-probe methods, optical, fluorescence and electron-beam microscopies, theory and modelling. Such a range of tools and techniques is not found in a single university department, and the purpose of the IRC is to ensure that there is easy access to what is required to tackle research problems that cut across the traditional departmental divides. In addition to representing the key disciplines in life and physical sciences and engineering, the principal investigators all have a proven record in successful inter-disciplinary research activity. There are a number of important and developing areas of research that are strongly represented among the investigators, and these will provide points of initial departure. However, we would want to be judged on our success in generating new collaborations and new approaches. As we detail elsewhere, we will keep a significant fraction of our budget to be bid from within the consortium, to support research projects that develop with time across the disciplines.

Materials systems which we will study include: molecular materials for electronics and photonics, building on the excellent UK standing in polymer electronics; self-assembly approaches to well-defined structures, including the investigation of fibril structures in proteins and polypeptides and their deposition or growth for use as structural components, wires or other nanodevices; and controlled cell growth from substrates for use as the basis for new materials for tissue engineering or in the creation of natural biosensors.

This ‘basic science’ nucleus of activity will be kept focussed, and will be aimed at encouraging curiosity-driven research. However, this will not be at the expense of relevance to **industry** and to **applications**. The natural point to transfer to an application-relevant approach is at the level of the materials systems studied. We identify at the outset two broad classes of ‘end-user’. The electronics/communications industry will benefit from the development of electronics and photonics with molecular or polymeric materials. Applications in the biomedical area will result from advances in tissue engineering and biosensor technology. The consortium includes a number of groups with strong track records in technology transfer, both with large organisations and also through company start-ups.

A final objective of the IRC is to plan for a significant lifetime well beyond the 6 years funding period requested. As evidenced in the letters of support from the Vice-Chancellors each University clearly sees nanotechnology playing a pivotal role in future strategies and development. The fact that each institution will establish a physical centre for the IRC, that nanotechnology is firmly placed as **the** technology for the next 20 years and that interdisciplinary research is becoming increasingly important all point to a healthy future for the IRC. There will undoubtedly be an organic growth of the IRC in the first 6 years as complementary funding develops. We would also expect the membership of the IRC to grow through such secondary funding. Successful commercial exploitation will also feed back into the IRC and provide a basis for a developing commercial relationship into the future. Finally, within each institution the ethos of interdisciplinary research and education will establish the role of the IRC in Under- and Post-Graduate education; support for these programmes will naturally need to extend beyond the initial 6 year phase.

3. Significance & Originality of Research

The presentation of the Objectives in section 2 above makes clear that grouping of science and engineering skills addresses the handling of molecular or biomolecular materials to form nanostructures with important functionalities, such as electronic or photonic properties, or biomolecular responses. Without being too prescriptive, or application-oriented, we have drawn from many discussions within the IRC grouping four **themes** which capture the philosophy of our approach, and which form a practical guiding framework within which we can organise disparate skills and starting points coherently. These four themes are: (1) Nanoscale fabrication and characterization, (2) Interfaces, (3) Directed Growth and Assembly, and, (4) Architectures and Devices. Themes (1), (2) and (3) are concerned with ‘extending the base of knowledge’ and theme (4) addresses the output from the work such as ‘... the quality of life and wealth creation’. We describe these in turn:

Theme 1 - Nanoscale Fabrication and Characterization

Introduction

The challenge for this research theme is to develop and harness a full range of complementary tools to enable the manipulation of atoms and molecules into desired morphologies, and then to interrogate their function and behaviour. The

techniques used to create, assemble and characterize structures at the nanoscale will involve a blend of existing, developing, and yet-to-be discovered technologies.

Manipulation and modification

The advent of scanning probe microscopy (SPM) has provided a set of tools for the direct nanomanipulation and modification of objects on surfaces. Switching between operational modes, an atomic force microscopy (AFM) tip can interchangeably image and move objects on a substrate, for example in manipulating single walled carbon nanotubes (SWNT), with the possibility of forming molecular interconnects or “wires” between components. Nanometre-scale SPM lithography is possible through the application of localized strain or electric fields (AFM and STM respectively). Nanoimprint lithography (NIL) and microcontact printing (μ CP) (so-called “soft lithographies”) provide novel routes to high throughput, low cost nanolithography. The success of these techniques will require expertise in polymeric materials and surface chemistry, qualities personified in this consortium. More conventional lithographies developed for microelectronics are being extended to fabricate new electronic nanostructures. High resolution electron beam lithography will be used to fabricate novel nanomagnetic structures yielding vast improvements in data storage and device integration density and polycrystalline nanowires. The integration of top-down physical and bottom-up chemical assembly methods as a route to novel nanostructures is aptly illustrated by the electron beam irradiation of organometallic cluster polymers to fabricate conducting nanowires. This interdisciplinary approach is essential for progress in nanoscale science, and provides a model for future developments in the proposed IRC. Similarly, at the interface of biology and physics, DNA chips and arrays are already in use in hybridisation assays. The potential exists to extend this technology to site-specific DNA-directed assembly of molecules.

Characterization

Electron microscopy will also be used to characterize nanostructures, with the use of photoemission to yield elemental information, holography to probe internal fields and environmental scanning electron microscopy for following colloidal aggregation processes. Spectroscopic SPM techniques now extend the scope of near-field optical microscopy beyond topography and into measurement of a plethora of local properties at the nanoscale. The ongoing development and refinement of non-contact transverse dynamic force microscopy (TDFM) in Bristol is providing a new suite of microscopes for non-invasive characterization of nanostructures, and the true 3-dimensional mapping of electric and magnetic fields. “Soft” polymeric and biomolecular nanostructures require “soft” imaging, and now full control of cantilever resonance is allowing low-force and nanometre resolution of these materials. This feature is essential for the non-invasive monitoring of the formation of nanostructures, for instance following the aggregation of amyloid fibrils as a precursor to novel biotemplates for nanostructure growth.

Relevance to other themes

Lithographies provide the templates from which directed growth and assembly can subsequently proceed, while well-developed characterization tools are essential to verify that desired structures have, indeed, been produced, and to aid in understanding the fundamental processes to be explored under the *Interfaces* theme.

Theme 2 - Interfaces

Introduction

The fabrication of nanometre-sized objects necessarily creates structures that have a much larger proportion of surface or interface than structures with larger dimensions. One of the challenges, therefore, for the field is to control, measure and model the properties of interfaces. Interfaces control the growth and structure of materials (for example, where a structure is grown off a substrate), and control electronic structure and electronic properties in many ‘functional devices’. In the context of the research themes for the IRC, the interface between inorganic (‘hard’) materials, with strong intermolecular interactions, and organic (‘soft’) materials, with weak intermolecular interactions, is particularly important. We illustrate below our approach to these challenges by reference to the research skills and interests within the consortium.

‘Tips on soft matter’

We consider our understanding of the weak intermolecular interactions at interfaces which do not involve strong chemical bonding to be central to the IRC, since this underpins many of our activities using molecular materials (biological or otherwise). Scanning probe microscopy is a very important experimental technique to the IRC, with strengths both at Bristol and Cambridge. The tip-sample interaction provides a useful model system for this interface, and we will explore this both by experiment and by modelling, both as a mechanical interface and as an electronic interface.

Electronic structure

Recent advances in polymer semiconductor devices (Light Emitting Diodes - LEDs - and Field Effect Transistors - FETs etc.) have lifted performance and application for these materials in semiconductor applications well beyond expectations set a decade or so ago. One of the fundamental reasons for this success is that the interfaces between molecular semiconductors and inorganic electrodes (for hole or electron injection in LEDs and FETs), and between different molecular semiconductors (heterojunctions), have proved to be much more controllable than expected. Quite generally, these interfaces do not produce electronic defect states which lie in the semiconductor gap, so that remarkably clean device performance can be achieved. This is in spite of substantial chemical modifications, which are well-known to form between, for example, thermally-

evaporated metals and molecular or polymeric semiconductors. These interactions are also central to the usefulness of inorganic semiconductor nanocrystals such as CdSe, which can be interfaced to form functioning semiconductor heterojunctions when mixed with semiconducting polymers.

Control of structure of soft matter grown on substrates

Differences between surface and bulk structures are well understood for inorganic materials such as metals and semiconductors. However, for soft condensed matter grown on a 'hard' substrate, there is less known about the influence of substrate on the local structure grown off it. This theme is important to the control of structure and properties of electronic devices made with molecular or polymeric semiconductors, and is important in the control and properties of biological structures, such as the conformation of proteins. Problems that we will address in this area include the control and characterisation of structures formed onto chemically-modified substrates (see *directed growth and assembly* theme), including both biological molecules formed onto novel substrates such as plastics, and electronically-active molecules as used in active devices.

Relevance to other themes

The fundamental understanding of mechanical and electronic properties of interfaces is the key to developing *architectures and devices* involving several different nanoscale components, and hence to the exploitation of *directed growth and assembly*.

Theme 3 - Directed Growth And Assembly

Introduction

The self-assembling nature of molecules and crystals provides a foundation for the manufacture of extreme nano-scale structures. However, self-assembly on its own is insufficient for most functional device development as the specific location as well as the structural form of the assembled object are key to the functionality of the system as a whole. This theme of the IRC is therefore aimed at developing techniques for directed assembly of nanostructures. There are two key aspects of directed growth and assembly: the placement of specific templates on which subsequent growth can take place; and the growth of structures from the templates.

Located Self-Assembly

Work on the location of specific templates will exploit the capabilities developed in the *Nanoscale fabrication and characterization* theme. These templates will be structures formed by conventional or other lithographic techniques, with some specific chemical attribute that enables subsequent assembled growth or attachment. Thus the primary requirement is for chemical recognition between the template and the structure to be grown from or attached to it, and although the template itself is likely to be a molecular structure, physical modifications such as texture or electronic excitation in the substrate may provide suitable templates.

Directed growth

From a template the growth may proceed in three dimensions; our research is aimed at developing techniques by which this growth may be directed. For example, the creation of a vertical rod from each template requires either that growth proceeds only in the z direction, or that structures self-assembled in the fluid phase attach vertically to the template. Similarly the attachment of macromolecules to template arrays will enable interconnected molecular surfaces to be formed. It is possible that alternative control techniques based on physical processes, such as electric field and structural anisotropy may become increasingly relevant.

Relevance to architectures and devices theme

The assembled object or structure may be functional in its own right, for example as a bioactive coating, but it can equally be a passive structure which forms the basis for further fabrication. This might involve further directed assembly, or lithographic steps.

Theme 4 - Architectures And Devices

Introduction

This area is central to the aim of the IRC because it provides the route by which the scientific themes of the collaboration will be harnessed to address technological needs. As we have stressed elsewhere, our key target in this proposal is the underlying science that can drive applications, rather than the applications themselves. Furthermore it is not appropriate to specify now, six years in advance, which devices or processes will be most ripe for development in 2007: not only is the path that our own technological development will take uncertain, but the external constraints and requirements are likely to have changed beyond all recognition in that time. Nevertheless, we have some clear ideas of the kinds of architectures we hope to develop during the project, and of their relationship to key functions in both information technology and biomedicine.

Example architectures

All these examples demonstrate the benefits obtainable from combining hard with soft matter, and molecular with inorganic materials; all involve strongly overlapping contributions from the different disciplines within the IRC.

- Fibrillar peptides in combination with electronically active components such as conjugated organic molecules, redox enzymes, or adsorbed metallic atoms, to produce novel highly one-dimensional conducting channels.
- Chemically structured organic films on lithographically structured 'hard' electrodes. This allows for the possibility of easily integrating organic and inorganic functions. The lithography and subsequent directed growth could proceed by any of the several processes outlined in the *nanoscale fabrication and characterization* and *directed growth and assembly* themes.
- Printable structures consisting of soft electroactive components on hard substrates. This could include structures produced by soft lithography or micro-contact printing, conferring controllable functionality on surfaces chosen for their other properties.
- Cholesteric structures or others that locally exploit molecular alignment for optical or electrical activity.
- Active components incorporated into artificial or naturally occurring membranes (e.g. 'rafts' of electroactive molecules incorporated into artificial micelles or into living cell membranes). These might be produced by exploiting two-dimensional phase separation of structures within such bilayers. These could include artificial channels for ions, or for other species.
- Specific coatings, aimed at controlling the biocompatibility or adhesion of organic or inorganic substrates in biological environments. These could include structures in which the adhesion-promoting properties of natural proteins (for example, immunoglobulin super-family domains or Arg-Gly-Asp/RGD peptide motifs), or of proteins specifically evolved for this environment, are combined with controlled structural rigidity from fibrils or from hard matter.

We expect progress during the IRC term to generate completely new perspectives, and we would therefore view the IRC as a failure if this list turned out to be a complete one.

Possible devices

The range of possible eventual applications for these structures, in information technology and in biomedicine, encompasses not only cases where the whole device is at a nanometre scale, but also where a larger (microscale or macroscopic) device depends on nanoscale phenomena and engineering to function. Here we give a small number of examples of such applications of the architectures; the list is of its nature incomplete, but indicates the potential scope and the absolute necessity of an interdisciplinary approach.

- Photovoltaic devices where the separation of charge is engineered using a combination of molecular chemistry and nanoscale patterning. Chromophores, charge donors and acceptors would be organised by directed assembly, and interfaces would be engineered allowing efficient charge transfer to an external circuit; this relies on knowledge of the underlying mechanical and electronic interactions.
- Photonic devices in which the spatial behaviour and coupling of electronic states and optical modes are controlled together. Block copolymers with varying refractive indices and electronic properties would be grown by directed assembly on surface templates to produce structures which are both optical waveguides and 'quantum wells' for carriers; to achieve this a fundamental understanding of excitations and their interactions is needed.
- Coatings that could be used to control cell adhesion to implants; ultimately such coatings might also be used to affect cell response to the local environment and so to control cell differentiation during tissue growth or other aspects of behaviour. The unique nanoscale contribution is to organise the coating on the macromolecular length scale, and to alter controllably its chemical and structural properties on the scale relevant to biological recognition, via development of new peptide-based structural components.

We can also envisage applications to nanoscale mechanical devices, storage devices (mechanical, electronic and magnetic), sensors (including biosensors), FETs, photodiodes and LEDs, and possibly to quantum information processing (by controlling the rates of decoherence in nanostructures).

4. Research Programme & Added Value of IRC

Grouping of activities. The IRC builds on great strength among the collaborating groups. However, research no longer fits into the division of research according to the traditional university departmental structures. The IRC will play a central role in re-directing research so as to transcend these artificial barriers. **We see that this IRC will play an important role in accomplishing this at the physical sciences – life sciences interface.**

At all three universities, IRC activities will be based around local centres, which will provide the extra resource needed to allow research to happen outside a single department (and, in the present context, university). These centres will be located at single sites at each Institution, on the West Cambridge site in Cambridge, at the UCL Centre for Nanotechnology once it becomes operational, and in the Physics Department at Bristol.) They will provide, firstly, space for visitors from other departments, so that all have 'right of access' to the centres, and so that there is provision for meetings. Secondly, although more specialist equipment will remain in the individual research groups, we identify a need to offer 'core' experimental facilities at the centres, to enable 'first look' experiments to be done without the need for full-blown cooperation between specific departments. Such facilities include techniques such as scanning-probe microscopies (AFM's), fluorimetry, optical microscopies, and some soft lithography.

The importance of this field is such that two of the universities involved (Cambridge and UCL) already have well-developed plans for infrastructural initiatives in this area. In Cambridge there is a commitment to organise nanoscience and

nanotechnology on a university-wide basis, and this will be centred eventually at the West Cambridge site (which at present comprises the Cavendish Laboratory, and in due course, Computer Science, Engineering and Materials Science). The Cavendish Laboratory identifies the theme of this IRC as top priority for its strategic research development. It will therefore assist in offering space sufficient to accommodate this IRC centre on the West Cambridge site, both for people and for equipment. This IRC space will be set up alongside space for Prof. Dobson (and other academic staff – one post currently advertised) to establish experimental biophysics in the Cavendish. This will also allow Prof. Welland to move his nanofabrication facility to the Centre on the West Cambridge site. The Centre for Nanotechnology to be established at UCL (which has committed one of the few remaining sites for building on its main campus) will integrate nanofabrication and characterisation tools for the research community in the physical and biomedical sciences.

The programme is divided into two very distinct types of activity:

First, there are **core projects** which will run for lifetime of the IRC and which will maintain the core competences at the three Institutions (and which will take place at the three Centres). This accounts for approximately one third of the man-months of research activity.

Second, there are **exploratory projects**, which will be shorter-duration activities, running from between a few months up to 3 years, and which will be selected from time to time in response to suggestions arising from within the three Institutions, either from the Management Committee, or from outside. Exploratory projects must involve direct activity from at least two University Departments, and may involve participation from outside institutions. The function of these exploratory projects is to draw in new ideas and new people. We see this as illustrating the character of our IRC as being outward-, not inward-looking. It is essential that management of the IRC is rapid and imaginative, so that new ideas can be picked up and run with very quickly. At the end of an exploratory project, we expect to see those that have grown to become large and self-sustaining to generate responsive-mode funding (some of which may plough back into the core technical competence of the IRC centres). This is an important route for planning the future viability of the IRC activities beyond the six-year lifetime of the assured core funding. Associated with each exploratory project is the provision for a **Studentship – 24 in total** to match the 72 man-years of exploratory project time projected.

Our exploitation strategy is the same for both types of project: where commercial possibilities are identified, the Management Committee will encourage technology transfer, to both large and small companies, making use of the Industrial Advisory Council.

We outline in detail **core** projects below.

Composition of the proposed IRC

The **seven investigators** will provide core organisational commitment to the IRC. Briefly their interests and roles are:

Prof. M. E. Welland (Cambridge, Engineering) Nanofabrication and characterization of structures and devices with unique electronic, optical and magnetic properties. Biosensors.

Dr. M. G. Blamire (Cambridge, Materials) Ion and electron beam device nanofabrication and characterization.

Prof. M. J. Miles (Bristol, Physics) Scanned probe microscopy of organic and biological materials.

Dr A.J. Fisher: (UCL, Physics) Theory of scanning tunnelling microscopy, and of coherent electron transport processes in molecular and atomic-scale conductors; development of electronic structure methods with open boundary conditions to treat transport in nanostructures.

Prof. R. H. Friend (Cambridge, Physics) Semiconductor physics of molecular and polymeric materials.

Prof. C. M. Dobson (Cambridge, Chemistry) Protein folding and misfolding, nanostructures formed by fibrillar proteins, biological devices.

Prof. M. A. Horton: (UCL, Medicine) Biological applications of nanotechnology, including the development of combined optical/scanning probe characterisation instruments and their use to image cellular processes.

In addition to the seven investigators, it is our clear intention to involve a significant number of other academic staff, whose contributions will be ordinarily through participation in exploratory projects. We have provided below a selection of representative exploratory projects, from which the Management Committee would select according for funding. This provides an initial list of other academic staff who have indicated their enthusiasm for the IRC and their willingness to participate. This list is necessarily a snap-shot (as of Jan. 2001), and we certainly expect and want to see others join, as appropriate, from time to time.

Other Academic Staff:

Dr. A. Alie	(Cambridge, Engineering). Fullerene-based electronics
Dr C. Abell	(Cambridge, Chemistry). SPM of single-molecule interactions at surfaces
Prof H. Ahmed	(Cambridge, Physics). Single electronics, e-beam lithography.
Dr Z. H. Barber	(Cambridge, Materials). Film growth for nanostructures.
Dr P. D. Barker	(Cambridge, Chemistry). Protein folding and crystallisation

Dr B. R. Bowler	(UCL, Physics) Development of 'linear-scaling' electronic structure algorithms for nanostructure growth and electron transport.
Dr F. Cacialli	(UCL, Physics) Application of SPM to conjugated polymer films and the construction of nanoscale devices for electronic and photonic applications.
Prof A. M. Donald	(Cambridge, Physics) Electron-microscopy, including ESEM, of soft condensed matter
Dr. C. Durkan	(Cambridge, Engineering) SPM of electronic materials and devices.
Dr C. Ford	(Cambridge, Physics). Low-temperature transport in low-dimensional electron structures, nanocrystal devices.
Prof M. J. Gillan	(UCL, Physics) Development of <i>ab initio</i> electronic structure techniques, including 'linear-scaling' algorithms and <i>ab initio</i> thermodynamics.
Dr N. C. Greenham	(Cambridge, Physics) Polymer semiconductor and nanocrystal electronics
Dr G. Hähner	(UCL, Physics) Scanning probe and photoemission studies of adsorbed organic films on surfaces, including understanding their interactions with biomolecules.
Dr D. Hasko	(Cambridge, Physics). Single electronics, e-beam lithography.
Prof A. B. Holmes	(Cambridge, Chemistry) Polymer chemistry, polymer electronics
Dr W. T. S. Huck	(Cambridge, Chemistry). Surface and macromolecular chemistry, soft lithography
Prof. B. F. G. Johnson	(Cambridge, Chemistry) Cluster chemistry, supramolecular structures for nanoelectronics
Dr L.N. Kantorovich	(UCL, Physics) Theory of ion scattering and scanning force microscopy; theory of defect states.
Prof. C. Lowe	(Cambridge, Institute of Biotechnology) Applications of biotechnology to sensors and devices.
Dr T.J. McMaster	(Bristol, Physics) Scanned probe microscopy of organic and biological materials.
Dr P.A. Midgley	(Cambridge, Materials) Electron microscopy and holography.
Prof. W. I. Milne	(Cambridge, Engineering) Amorphous carbon and silicon based electronic devices.
Dr T. Rayment	(Cambridge, Chemistry) SPM of single-molecule interactions at surfaces. X-Ray crystallography.
Dr A.L. Shluger	(UCL, Physics) Theory and interpretation of Scanning Force Microscopy; theory of localized excited states at surfaces and their effect on materials modification; theory of defects and their excitations.
Dr. H. Sirringhaus	(Cambridge, Physics) Polymer electronics, direct printing of functional structures, BEEM spectroscopy
Dr M. Sprik	(Cambridge, Chemistry) Development of <i>ab initio</i> molecular dynamics methods to treat environmental effects in chemical reactions in solution.
Prof A.M. Stoneham	(UCL, Physics) Theory of scanning probe microscopy; theory of materials modification by excited states; control of thin-film growth and defect structures; theory of condensed-phase quantum computation; influence of mesostructure on macroscopic electrical properties of conjugated polymers.
Dr E. Terentjev	(Cambridge, Physics) Polymer theory and experiment, cholesteric elastomers
Dr M. Warner	(Cambridge, Physics) Theory of polymers, liquid crystals, complex fluids

Core Projects.

1. Nanofabrication and patterning [Cambridge].

The ability to fabricate structures with nanometre precision is of fundamental importance to any exploitation of nanotechnology. In particular, cost effective methods that are able to fabricate complex structures over large areas will be required. Our response to this is the establishment of a comprehensive core project at Cambridge double the size of the standard core project. By bringing together all the methods of fabrication into one project efficient use of resources and a coherent approach towards Nanofabrication issues will be assured. Our current list of topics include:

a) Patterned self-assembly for pattern replication

The aim of this project is to exploit e-beam and focused ion beam lithography to pattern self-assembled monolayers into 10-20 nm features that can be functionalised with single molecules or small molecular groupings. These patterned areas will then be used as templates to direct the vertical assembly of stacks of molecules or to direct the growth of polymeric molecules. The initial 2D pattern will thus be translated into 3D nano-sized objects. As we have full control over the interfacial properties, it will be possible to release the objects from the templates and transfer them to another substrate, after which the nanopatterned surface can be used again to provide an inexpensive replication technique.

b) Stencilling of complex structures and materials.

We have recently shown that the use of a lithographic shadow mask technique can produce a completely new range of structures. The principle is that a mask, which is actually a specially designed AFM cantilever with an array of holes, is moved over a surface with sub-nanometre precision whilst evaporating a number of precursor materials through it.

Complex 3D structures can be built directly without the need for conventional lithography. Such structures can be heated to effect a chemical reaction in a confined volume. We have used this method to produce the first extended single crystals of carbon nanotubes. The ability to place the nanotubes at precise positions on a surface is unique to the method and will allow for the construction of complex carbon based structures for electronic and mechanical applications. We will develop this technique to provide even greater precision in controlling the position and complexity of structures so that a new range of nanostructured materials can be exploited.

c) Device fabrication by direct printing.

This project will draw on recent advances in printing techniques for direct patterning of surfaces, and will build on the demonstration of all-printed, all-polymer transistor circuits reported recently by the Cambridge group. This involves the use of ink-jet printing to deliver a functional material (semiconductor or metal) to a substrate, which is then controlled by patterning in the surface free energy of the substrate, to allow very accurate patterning of the printed material. Currently, devices show channel lengths down to 5 μm , but indications are that geometries can be reduced to sub-micron dimensions. The project will be concerned with the limits to resolution that can be achieved by this process, and also the structure and associated electronic structure at polymer-polymer interfaces, such as that between semiconductor and insulator layers in the field-effect device.

d) Nanopatterned SAMs as 2D templates for 3D fabrication

Modern lithographic techniques (e-beam or focused ion beam (FIB), SNOM lithography) are able to generate topographic (relief) patterns in the 10-50 nm size ranges. As a further step towards more complicated and functional 3D structures, chemical functionalization at a similar size scale is necessary. We propose to exploit e-beam, FIB and near-field optical lithography to pattern self-assembled monolayers *directly*. Using lithography, the SAMs can either be locally destroyed and refilled with other molecules, or the surface of the SAMs can be activated to allow further chemical reactions. The resulting patterned surfaces will be chemically patterned. We can introduce patterns that incorporate H-bonding, pi-pi stacking, or chemical reactivity. These patterned areas will be used as templates to direct the vertical assembly of stacks of molecules or to direct the growth of polymeric molecules. Large, extended aromatic molecules prefer to stack on top of each other due to pi-pi stacking. These molecules have interesting electronic properties as molecular wires. When surfaces can be patterned to incorporate 'seeds' for the large aromatic molecules, the stacking can be directed away from the surface. The initial 2D pattern will thus be translated into 3D nanosized objects. As we have full control over the interfacial properties, it will be possible to release the objects from the templates and transfer them to another substrate, after which the nanopatterned surface can be used again to provide an inexpensive replication technique.

e) Novel resists and resist processes.

Current microelectronics production depends on highly-sensitive and high resolution polymeric-based resists. The scaling of devices will soon be limited by currently-available resist behaviour, for example associated with the inherent disorder in spin-coated polymer resist layers. This project will develop measurements and processes to understand structure at the molecular scale, in order to develop new ways to pattern, for example by selective dissolution of material patterned by a range of techniques including e-beam, STM, optical and microcontact printing. Measurements include viscoelastic and other thermodynamic properties of polymeric thin films, using AFM and ultrasound. Control of interfacial surface structure, and the use of self-assembling polymeric structures will be developed in parallel.

f) Pattern transfer from thin resist layers

Decreasing lengthscales have traditionally required the use of progressively thinner polymer resist structures. A method of transferring such patterns into deep heterostructures has usually been to use composite resist structures in which a thicker organic or inorganic material is patterned using the initial thin coating in order to serve as a more robust mask. There are obvious limitations to such a process and considerable research has been directed to overcome them. One method by which a thin resist structure may be more faithfully transferred to secondary resist structure is by exploiting crystallographic or microstructural texture to enhance etch rate anisotropy. Several techniques for the promotion of texture on untextured substrates are already under development for the deposition of functional coatings with improved performance including oblique laser ablation and self-shadowing deposition. The aim of this project is to apply similar techniques for the creation of secondary inorganic and polymer resist structures and to optimise their growth and patterning. Suitable developers with high diffusivities, selectivity and adjustable solvating power are needed for the rapidly shrinking feature sizes of microelectronics, and considerable promise lies in polymer processing in supercritical carbon dioxide. Success in this project will allow deep-nanoscale patterning to be applied more generally.

Investigators and collaborators: Prof. M.E. Welland, Dr. C. Durkan, Dr. W. T. S. Huck, Dr. M.G. Blamire, Dr. H. Sirringhaus, Prof. R. H. Friend, Dr. D. Hasko, Prof. H. Ahmed, Prof. B. F. G. Johnson, Dr. Z.H. Barber, Prof. A.B. Holme, Dr. F. Cacialli.

2. Characterization of Nanostructures by SPM [University of Bristol]

A core project is concerned with the development and application of scanning probe microscopy for the characterisation of structures and functions of nanostructures developed throughout the IRC. The SPM techniques that will be applied include AFM, STM, SNOM, non-contact shear-force microscopy and force spectroscopy. These techniques must be capable of imaging soft organic and biological specimens in various environments including liquid. In addition to these 'standard' techniques, the active-Q technique implemented on AFM is of particular importance for decreasing the applied force and

increasing the phase contrast in liquid environments. The transverse dynamic force group of microscopes (TDFM), of which ShFM is one example, can be used to characterize magnetic (or electric) fields in 2 and possibly 3 dimensions. TDFM can also be used to provide force vector information in force spectroscopy measurements. A very recent development is the possibility of imaging on the millisecond timescale. This technique will be used to monitor the assembly of the nanostructures in appropriate cases and to observe function such as recognition processes or molecular motion. A wide range of SPM instrumentation will be dedicated for use in collaboration with members of the IRC. The more novel techniques will require ongoing development.

Investigators and collaborators: Prof. M.J. Miles, Prof. M.E. Welland, Prof. R. Friend, Prof. M. Horton, Dr. Cacialli, Prof. C. Lowe, Prof. C. Dobson, Prof. B. Johnson, Prof. A.M. Donald, Dr. T. Rayment,

3. Smart Bio-Materials [UCL]

One of the most pressing medical needs is to develop new materials that will drive and maintain a required and appropriate cellular and tissue response. These will be used in the replacement of degenerating and diseased organs and tissues, conditions that affect millions of individuals in our ageing society and cost health services £ billions annually. Advances to date have largely been empirical, and measured outcomes often rely on direct testing in patients (e.g., joint or vascular prostheses, tissue engineered cell implants). The knowledge base acquired from the 'bottom up' approach to be utilised within the IRC provides an opportunity to break this mould and design new materials – protein or chemically based – *ab initio*. Materials will be produced in a regulated way, based upon nanoscale information obtained from fundamental techniques and theory, for the assembly of organic components; moreover, they will exhibit properties that are controllable (e.g., by electrical, electrochemical or mechanical transduction to modify/produce chemical entities in patterned SAMs). Specific coatings for biomedical applications - aimed at bio-compatibility, adhesion or other biological functions - will be created and evaluated based upon the 'amyloid fibre' strategy to form protein-based materials of defined and controlled structure and deposited with nanoscale precision. These 'smart bio-materials' could eventually be used to control cell adhesion, say to orthopaedic or vascular implants, and to control cellular responses and behaviour in the local environment during tissue repair.

Adhesion promoting features of natural proteins will be utilised as modules for the creation of stable fibres. Examples could be from extracellular matrix or other protein domains that contain RGD peptide sequences that interact with cell membrane integrin receptors (such as the 10th type III repeat in fibronectin or the snake venom protein echistatin). Interactions between immunoglobulin superfamily domains that are naturally involved in cell-cell interactions could also be utilised (for example, the Ig domains of CD2 and LFA3 to control local immune function). The support structure would have its surface topography and chemical characteristics controlled to bind and orientate the fibres and to form 'mats', which in turn would exhibit their own (controllable) nanoscale topography. Naturally occurring motifs in the protein modules could be manipulated genetically or new ones, such as chemically synthesised 'drugs', could be added during fibre formation. Cellular responses could also be regulated by adding further modules containing growth factor functions (such as VEGF to regulate vascular proliferation) as illustrated.

The fibres so deposited will be characterised at various length scales to investigate fibre morphology; functional motif distribution in the repeat units of fibres; their mechanical properties and chemical stability; the nature and control of changes in chemical/functional properties induced at the hard-soft boundary; the interaction forces between the material surfaces and deposited the matrix proteins and cell membranes which define their biological specificity; and the 'phenotype' of the tissue response to the materials in proof of concept *in vitro* cell culture experiments. Many of the characterisation methods that will be used in this core activity will be those techniques developed and performed on the chemically and lithographically produced surfaces produced elsewhere in the IRC.

Investigators and collaborators: Prof. M.A. Horton, Dr G. Hähner, Dr F. Cacialli, Prof. C. Lowe, Prof. C. Dobson, Prof. M.J. Miles.

4. Computational methods for molecular nanotechnology [UCL]

The computational and theoretical projects within the IRC will rely on the development of core techniques to address several key problems. One is how to treat quantum mechanically systems in contact with an environment - in particular when there are open boundary conditions that allow particle exchange between the system and the environment. This is important because such open boundary conditions are ubiquitous in nanotechnology: molecular systems are generally in intimate contact with their environment and are often required, in applications, to carry a current. A second question involves the inclusion of the dynamic effects known to be involved in electron transport. While we now appreciate their importance and can include their effects in simple cases, our existing algorithms scale badly with system size and new approaches are needed. A third important question is how to treat effectively electronic excited states in their nanoscale environment.

Providing these capabilities is not a question of code maintenance: it requires much genuinely new science, as well as high-quality code development. We have an excellent base of code to build on, much of it developed 'in-house'. This code base includes the CONQUEST code (a highly parallel $O(N)$ *ab initio* electronic structure code capable of calculations on tens of thousands of atoms); its structure and underlying methodology make it readily adaptable to these nanoscale problems. We also have specialised codes for the treatment of electron-phonon coupling, for STM and AFM image simulation, and for the embedding of excited states.

We will maintain close contact with others involved in taking forward related ideas, notably with the CCP1 collaboration, where a project led by Dr M. Sprik is focussed on including the environmental effects of aqueous solvation on reaction dynamics calculations in solution.

Investigators and collaborators: Dr A.J. Fisher, Prof. M.J. Gillan, Prof. A.M. Stoneham, Dr A.L. Shluger, Dr D.R. Bowler, Dr M. Sprik.

5. Environment

The support requested for the IRC will build on a strong base of research activities in the three Institutions. All 7 investigators have strong research support, from the Research Councils, from the European Commission, and from industry. The other named academic staff also have strong and well-supported research programmes. The total research activity covered by these two groups is considerably larger than the activity that will be supported directly by the IRC programme. The purpose of the IRC is to build onto this strong research base the extra structures that will enable cross-disciplinary activities in nanotechnology. We have identified the need for physical centres at each Institution that provide equipment and know-how for the basic nanotechnology activities which allow new projects to get started with the minimum of formality, but we do not intend that these centres absorb the more specialist techniques (particularly for measurements) which currently reside within individual academic staff groups. We expect to be judged on the extent to which we have created this extra dimension to the activities at the three Institutions. Our intention is therefore not to support 'gaps' in research funding, nor is it to replace 'responsive mode' funding with IRC funding.

We have detailed above the seven investigators and also a starting list of other named academic staff. These other staff will have access to the IRC facilities, through participation in either **core** or **exploratory** projects and their involvement is central to the purpose of the IRC; clearly evident from their association with both core and exploratory projects detailed in section 4.

The creation of the three IRC centres at the three Institutions will clearly require new space, and all three Vice-Chancellors commit to this. A range of funding sources including SRIF and industrial will be used for this.

The role of industry is discussed below within the context of exploitation and technology transfer. However, industry plays a very important role in the direct support of research, either through funding, or, equally importantly, through access to technology. It is therefore very important that we take advantage of this support within the IRC. The investigators and other named staff collectively have excellent links with a wide range of industrial organisations. We see these links as the natural points of contact between the IRC and industry, and will encourage industrial support of IRC projects (both core and exploratory). However, this will not be at the expense of open communication within the IRC, since open discussions, unfettered by proprietary considerations, must be the engine of new directions and new projects. We recognise that industrial organisations will also value access to information about the whole programme of activity within the IRC, and we will set up an **industrial club**, with membership drawn initially from those organisations that do support IRC research. This industrial club will receive a regular newsletter detailing activities in the IRC, and will be invited to regular review meetings at the IRC.

6. Management

As described above, the IRC is split between three establishments, and it is essential that a clear and robust management structure is established. We note that at each establishment, a physical centre will be established, at which the local activities will be coordinated, and between which, the 3-centre coordination can be accomplished clearly and effectively.

The IRC will have a **Director**, and Professor M. E. Welland (Cambridge) is designated for this role. He will move all his research activities from the current Engineering Department buildings on Trumpington Street to the new centre on the West Cambridge site. His activities will be fully directed towards the operation of the IRC. Professor Welland's role as IRC Director has the full support of the University. The successful establishment of the IRC on the West Cambridge site forms a vital part of the Engineering Department's development plans. The **Director** will chair the **Management Committee**, which will comprise:

Professor M. E. Welland (Cambridge)
Professor M. Miles (Bristol)
Dr. A. Fisher (UCL)
Professor R. H. Friend (Cambridge)
Professor C. M. Dobson (Cambridge)
Professor M. Horton (UCL)

This Management Committee, or subset of it, will meet at least six times a year. It has the function of managing the scientific direction of the IRC internally and externally, and of managing the resources of the IRC. As discussed above, the IRC budget will be split into two components; the first is 'core' support to provide the essential infrastructure at each Centre, and the second is project support. These will be bid for within the consortium and allocated by the management committee. All projects will involve more than one discipline, and would normally require that post-docs funded in this way held joint

appointments at more than one department. The Management Committee will be responsible for the allocation of this project support.

Resource allocation between Centres will therefore be clearly established, and local management at each Centre of these resources can therefore be effective. However, responsibility to ensure that activities throughout the IRC are effective and coherent rests with the Director, and he will make use of the Management Committee to assist him in this task.

In addition to the Management Committee, two further committees will be set up, an **International Scientific Advisory Council** to assist the Director in establishing that scientific quality and direction are internationally competitive, and an **Industrial Advisory Council** which will provide contacts and advice on contacts with industry and exploitation. This latter Committee is discussed further below: Commercial Exploitation and Technology Transfer. The **International Scientific Advisory Council** will be formed from a number of leading international scientists (not UK-based), who will be invited to an annual report and meeting at which they will have the opportunity to observe and criticise the operation of the IRC.

The International Scientific Advisory Committee provides an important means for ensuring that the IRC has a high international profile. The Director will have the responsibility to promote the IRC nationally and internationally, and this is fully consistent with his high international profile. In doing this, he will also draw on the other Investigators who are also frequently invited to national and international meetings.

It is recognised that the Director will have a very heavy load in setting up and managing the IRC. This will be taken into account in the teaching and other duties that the Department will require of him. He will keep a reduced lecturing load (since exposure to undergraduates of this area of science and engineering is an important aim of the IRC). Where appropriate, Professor Welland will pass executive responsibilities to other members of the Management Committee (for example, local management at Bristol and UCL).

The IRC at all three institutions will be well-supported by existing administrative systems, and will have direct and ready access to technical support. Within each University, there is considerable experience in the operation of cross-departmental research. For example, Cambridge has learned much from the operation of the IRC in Superconductivity, which was set up (as required by the SERC) as an Institute separate from the participating departments. This independent status has now been removed, and a more flexible system introduced, in which one of the university departments (Physics) provides infrastructure support, but the IRC research activity retains independence (though answerable to the Councils of the Schools of Physical Sciences and of Technology). This model is working well, and will be used as the basis for the nanotechnology IRC.

The three institutions will use well-established policies for the distribution of indirect costs on grants held by researchers within the IRC, with distribution between central university, local university department, and the investigator. By operating the IRC within the existing departmental structures of the three Institutions, many of the problems which have arisen in the past, for example, associated with the distribution of HEFCE support in respect of teaching, are avoided.

7. Training & Development

Students will be expected to interact broadly within the IRC, learning a range of skills. No student will spend their entire PhD in a single department. During the 1st year in particular, students will move between groups to learn the different experimental/analytical/computational approaches relevant to their project and the different languages characteristic of the various contributing disciplines. This first year training will include attendance at a range of short courses on relevant topics, to ensure that students do not become too narrowly focussed. Because of the multidisciplinary nature of the research, we envisage operating within the EPSRC's new flexible training accounts, with 4 years as the standard duration for a PhD within the IRC, to provide the time needed for proper training. Annual student day(s) will be arranged at which all students will be expected to make presentations to other IRC members (including the industrial management committee) to ensure both dissemination of information between institutes and (with feedback provided) the development of professional oral communication skills. Written end of year reports will develop the corresponding written skills. The interdisciplinary nature of this field makes communication training vital: with such regular monitoring we can be sure our students will leave with a battery of employable skills to make them attractive to the SME's who will be carrying forward the exploitation of our research base.

The Entrepreneurial Centre sited at West Cambridge will provide ready access to short courses on Intellectual Property, formulating Business plans, identifying exploitation routes and running start-up companies. This important training element will be open to all members of the IRC.

We envisage establishing a series of Undergraduate courses relevant to the research activity of the IRC. Such cases are easily assimilated into the flexible structure of 4-year degrees currently offered at all participating institutions. Such courses will be designed to be transportable between IRC members so that a coherent Undergraduate training package will evolve.

In partnership with the Institute of Nanotechnology, see below, we will offer regular Workshops and Summer Schools – the first of which is planned for the Summer of this year – open specifically for education of researchers.

8. Commercial Exploitation & Technology Transfer

The IRC in Nanotechnology is intended to be a driving force in discovery and invention in new areas of research. This 'basic science' nucleus of activity will be kept focussed, and will be aimed at encouraging curiosity-driven research. External contacts will play a very important role in driving these research ambitions, and industrial contacts are particularly important. The IRC will develop many such industrial contacts, but will build these around the central structure of the IRC, ensuring that these contacts encourage open research. Among the investigators, and other staff expected to play active roles in the IRC there are many excellent links with industry, both with large companies and with smaller companies, and it is intended that these contacts provide the starting points.

In addition to the role of industry in furthering research, contacts with industry play a very important role in supporting commercial exploitation, and these research-oriented links will play these dual roles. It is always difficult to guess what will turn out to be commercially important, but at the outset two broad classes of 'end-user' are identified. The electronics/communications industry will benefit from the development of electronics and photonics with molecular or polymeric materials. Applications in the biomedical area will result from advances in tissue engineering and biosensor technology.

The IRC views the scope for commercial exploitation to cover both large corporates and also small, or start-up companies. Particularly in this area of nanotechnology, commercial applications often do not match the product portfolio of corporates (particularly if restricted to the UK, and even to Europe), and in this situation, a start-up company is now considered to be the preferred exploitation route. Within the Cambridge area, several start-up companies have grown spectacularly quickly in the past few years (e.g. ARM, AutoNomy), and are seen to be an increasingly important means for growing the high-technology base of the UK. There is considerable experience in start-up activities among the Investigators, and Cambridge in particular has now an excellent local base of know-how and VC funding. Several of the Investigators have direct experience of company start-up (e.g. Cambridge Display Technology), and will provide active assistance in this mode of technology transfer.

The IRC will therefore build in strong relationships with these small-company oriented activities, in addition to more traditional links with corporates. The IRC will set up an **Industrial Advisory Council** with membership drawn broadly from VC fund managers, research managers, and senior executives in industry. A tentative list of members includes:

9. Dissemination of Research Results

Standard procedures to ensure that patents are filed before publication will be followed at each of the three Institutions. In addition we have established an alliance with the Institute of Nanotechnology who will be specifically charged with disseminating results from the IRC to researchers, industrialists and the public. Please refer to section 13 below for full details.

10. Public Understanding of Science

The proposed IRC will work with the Institute of Nanotechnology (<http://www.nano.org.uk>) to achieve as wide an international audience as possible for the scientific and technological advancements achieved through the Centre's work. The IRC will also benefit from the Institute's commitment to informing the general public about nanotechnology, as a vital component in ensuring continuing acceptance of this new branch of science.

The Institute, which grew out of the UK's National Initiative on Nanotechnology (NION), has a long history of successfully promoting nanotechnology research to industry through conferences, workshops, publications and via its award-winning website. The Institute has also recently inaugurated its European Board (http://www.nano.org.uk/euro_board.htm), and this will provide additional scope for the dissemination of information.

The IRC can also become actively involved in making contact with the investment community through the Institute. A key objective of the IoN in 2001 is to prime investors regarding the potential of nanotechnology, through various awareness-raising events (<http://www.nano.org.uk/invest.htm>), with the aim of paving the way to informed investment, generating new companies and thus accelerating a return on research funding to the UK plc.