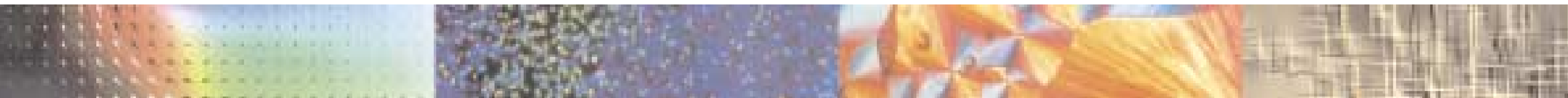
# OxfordMaterials

## Research in Progress

## 2006 - 2007



Department of Materials

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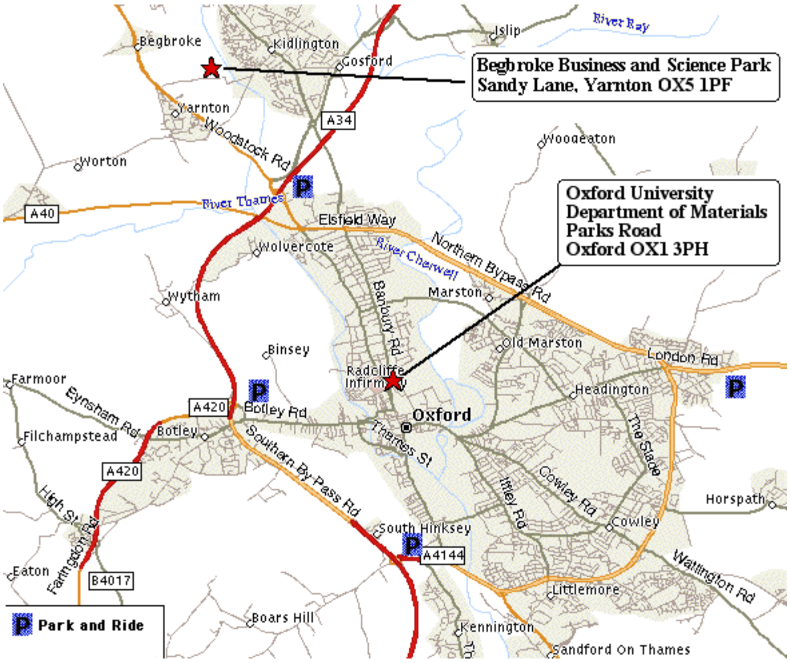
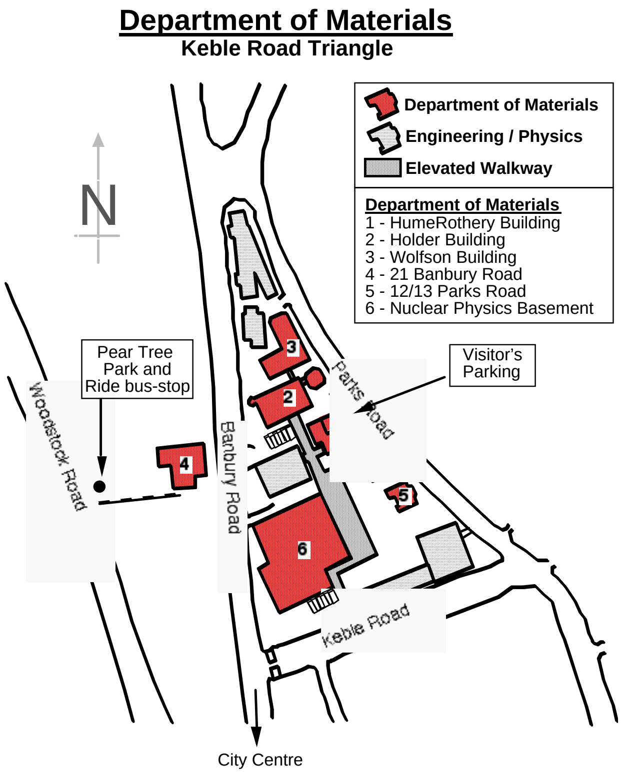
# Department of Materials

# University of Oxford

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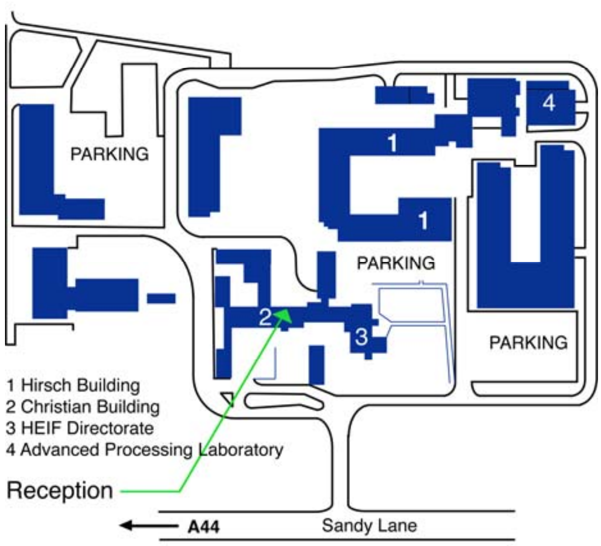


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# Foreword from the Head of Department

Welcome to this information on the Department of Materials at Oxford University. Our objectives are to produce world class graduate materials scientists and engineers, and to conduct world class research into the manufacture, structure, properties and applications of materials for the benefit of the UK and world community. We were awarded the highest "five star star" grading for research in the government's most recent assessment exercise, and we consistently top the overall performance league tables for UK Materials Departments.

The Department was founded by Professor Hume-Rothery in 1956. At present, it consists of 22 academics, 29 senior researchers, 50 postdoctoral researchers, 38 technicians and administrative staff, 64 academic visitors, and about 80 research students and 100 undergraduates. The Department is part of an integrated Division of Mathematical, Physical and Life Sciences at Oxford, which includes physics, chemistry, computing and engineering departments, providing an ideal environment for interdisciplinary teaching and research. Fundamental developments in the physics and chemistry of materials can take place directly alongside applications in manufacturing processes and engineering design.

Major achievements in recent years include:

1. Five elections to Fellowships of the Royal Society (David Cockayne, John Pethica, Brian Eyre, John Hunt and Adrian Sutton) and three to the Royal Academy of Engineering (Richard Brook, Brian Cantor and Amanda Petford-Long);

2. Awards and honours to members of the Department include; the Royal Society Armourers and Brasiers Award (David Pettifor, John Hunt), the Royal Society Hughes Medal and the IofP/SFP Holweck Medal and Prize (John Pethica), the Institute of Materials Platinum Medal (John Martin, Brian Cantor, George Smith), the Acta Materialia Gold Medal (George Smith), the Beilby Medal and Prize (Alfred Cerezo), the Pfeil Award (Richard Todd), the IOM3 2005 Alan Glanville Award (Hazel Assender). Metrology for World Class Manufacturing Awards (Andrew Briggs, Oleg Kolosov, John Hunt), the National Award for Innovative Measurement (Alfred Cerezo, Terence Godfrey and George Smith). In addition, Sir Peter Hirsch FRS was elected to the US National Academy of Engineering and to the American Association of Arts and Sciences as a foreign Honorary Member, and awarded the Heyn-Denkmunze prize of the German Materials Society and the Russian Academy of Sciences Lomonosov Large Gold Medal in 2005. Brian Cantor was appointed Vice-Chancellor of the University of York, Richard Brook received a knighthood, and was appointed Director of the Leverhulme Trust, David Pettifor was appointed a CBE for Services to Science, Andrew Briggs was appointed as the Director of a new Quantum Information Processing IRC, John Hutchison was elected President of the Royal Microscopical Society and David Cockayne was elected President of the International Federation of Societies of Microscopy (2003-6);

3. Appointment of Andrew Briggs to the Professorship of Nanomaterials and Patrick Grant to the Cookson Professorship of Materials;

4. Three promotions to personal professorships (Chris Grovenor, Steve Roberts, Angus Kirkland) and four promotions to readerships (John Hutchison, Mike Jenkins, Peter Wilshaw and John Sykes);

5. Over £8m from the Joint Infrastructure Fund, to purchase cutting edge equipment for atomically engineered, nanoscale materials processing and analysis;

6. The launch of the new £35m Begbroke site, which greatly expands the Department's space, and sets up a unique combination of industry-linked materials research and spin-out science park;
7. The establishment of the Faraday Advance partnership in aerospace and automotive materials;
8. The establishment in the Department of the main hub of the new £9.2m IRC in Quantum Information Processing. This follows the award of a £3.4m DTI Foresight Link grant for research on nanoelectronics and quantum computation.

The Department of Materials at Oxford provides a vibrant and stimulating environment, and acts as an academic meeting point for materials scientists and engineers from all over the world. This booklet describes the full range of our current research programmes. We are always pleased to discuss our research projects in more detail and to explore further opportunities for collaboration and scientific exchanges. We actively seek applications from new undergraduates, research students and research fellows from all over the world. Please do not hesitate to contact us by letter, phone, fax or e-mail.

Professor C.R.M. Grovenor
October 2006

# Members of Department

## Professors

| | |
|---|---|
| Professor C.R.M. Grovenor | *Head of Department* |
| Professor D.G. Pettifor, FRS | *Isaac Wolfson Professor of Metallurgy*<br>*Director of the Materials Modelling Laboratory* |
| Professor P.S. Grant | *Cookson Professor of Materials*<br>*Director of Faraday Advance* |
| Professor D.J.H. Cockayne, FRS | *Professor in Physical Examination of Materials* |
| Professor G.A.D. Briggs | *Professor of Nanomaterials*<br>*Quantum Information Processing Interdisciplinary Research Collaboration* |
| Professor A. Cerezo | *Professor of Materials* |
| Professor A.I. Kirkland | *Professor of Materials* |
| Professor S.G. Roberts | *Professor in Materials* |
| Professor G.D.W. Smith FRS | *Professor of Materials* |
| Professor C. English FREng | *Visiting Professor* |
| Professor J.B. Pethica, FRS | *Visiting Professor* |
| Professor C.R. Whitehouse | *Visiting Professor* |
| Professor J.V. Wood FREng | *Visiting Professor* |
| Professor Sir Richard Brook, OBE FREng | *Emeritus Professor* |
| Professor Sir Peter Hirsch, FRS | *Emeritus Professor* |
| Professor J.D. Hunt, FRS | *Emeritus Professor* |
| Professor M.J. Whelan, FRS | *Emeritus Professor* |

## Readers

| | |
|---|---|
| Dr. M.L. Jenkins | *Director of Electron Microscopy Facilities* |
| Dr. J.L. Hutchison | *Reader in Materials* |
| Dr. J.M. Sykes | *Reader in Materials* |
| Dr. P.R. Wilshaw | *Reader in Materials* |

## Lecturers

| | |
|---|---|
| Dr. H.E. Assender | *Lecturer in Materials* |
| Dr. M.R. Castell | *Lecturer in Materials* |
| Dr. J.T. Czernuszka | *Lecturer in Materials* |
| Dr. P.D. Nellist | *Lecturer in Materials* |
| Dr. K.A.Q. O'Reilly | *Lecturer in Materials* |
| Dr. J.M. Smith | *Lecturer in Materials* |
| Dr. R.I. Todd | *Lecturer in Materials*<br>*Director of Oxford Centre for Advanced Materials and Composites* |
| Dr. A.J. Wilkinson | *Lecturer in Materials* |

## Administration

| | |
|---|---|
| Ms A.P. Davies | *Administrator* |
| Mr T.P. McAree | *Deputy Administrator (Finance)* |
| (Dr. L.J.F. Jones) Dr. K. Dickers | *Deputy Administrator (Academic/Personnel)* |
| Dr. I.C. Stone | *Deputy Administrator (Academic/Finance)* |
| Dr. A.O. Taylor | *Director of Studies* |

## Senior Research Fellows

| | |
|---|---|
| Dr. R. Ball | Wolfson Industrial Fellow |
| Dr. A.S. Barnard | Glasstone Fellow |
| Prof. A. Balazs | OCAMAC Senior Fellow (Pittsburgh) |
| Dr. S.C. Benjamin | Royal Society Research Fellow |
| Dr. R. Bhatti | Senior Visiting Fellow (QinetiQ) |
| Dr. C. Bishop | Career Development Fellow |
| Dr. G.R. Booker | OCAMAC Senior Fellow |
| Dr. J.A.A. Crossley | Senior Research Fellow |
| Dr. R. Drautz | MML Research Fellow |
| Dr. S.L. Dudarev | OCAMAC Industrial Fellow (UKAEA) |
| Professor B.L. Eyre | Senior Visiting Fellow |
| Dr. R. Falster | OCAMAC Industrial Fellow (MEMC) |
| Dr. M. Galano | Career Development Fellow |
| Dr. N. Grobert | Royal Society Research Fellow |
| Dr. B. Gilmore | Senior Visiting Fellow |
| Dr. D. Imeson | Senior Visiting Fellow (DSTL) |
| Dr. C. Johnston | Senior Research Fellow |
| Dr. A. Kohn | RAE Research Fellow |
| Dr. B.W. Lovett | Royal Society Research Fellow |
| Dr. J.W. Martin | OCAMAC Senior Fellow |
| Dr. Duc Nguyen-Manh | OCAMAC Industrial Fellow (UKAEA) |
| Dr. P.J. Northover | Senior Research Fellow |
| Dr. S.C. Speller | RAE Research Fellow |
| Professor M. Stoneham | Senior Research Fellow |
| Dr. J.M. Titchmarsh | Senior Visiting Research Fellow |
| Dr. D. Vesely | OCAMAC Senior Fellow |
| Dr. P.D. Warren | OCAMAC Industrial Fellow (Pilkington) |
| Dr. A.A.R. Watt | Career Development Fellow |

## Research Fellows

Dr. D.E. Browne
Dr. V. Burlakov
Dr. A.M. Cock
Dr. L. Chang
Mr. F. Cullen
Dr. G. Dentelle
Mr. R.C. Doole
Dr. C. Dwyer
Dr. R. George
Dr. A. Gianattasio
Mr. T.J. Godfrey
Dr. T. Hammerschmidt
Dr. B.M. Henry
Dr. C.J.D. Hetherington
Dr. Y. Huang
Mr. D. Hutton
Dr. K. Jurkschat
Dr. K. Kohary
Dr. P. Kok
Dr C Lang
Dr. V. Lazarov
Dr. X. Li
Dr. S. Lozano-Perez
Dr. J. Mi
Dr. G. Moldovan
Dr. R. Nicholls
Dr. R. Novokshanov
Dr. K. Porfyrakis
Dr. M. Ratoi
Mr. C.J. Salter
Dr. M. Schröder
Dr. S. Senkader
Dr. G. Sha
Dr. F. Silly
Dr. J. Topping
Dr. J.H. Warner
Dr. P.J. Warren
Dr. L. Xiao
Dr. Z. Yao
Dr. C-Y. You
Dr. R.M.K. Young

## D.Phil and MSc. Research Students

Abraham, M.H. (self-supporting)
Aggarwal, N (EPSRC)
Ahmed, S. (CASE: Corus)
Alpass, C. (EPSRC DTA)
Armstrong, D. (EPSRC DTA)
Bagot, P. (EPSRC)
Banjongprasert, C. (Thai Gov.)
Barkhouse, A (Rhodes Scholarship)
Beal, R. (Rhodes)
Behan, G. (Department / Intel)
Britz, D. (EPSRC Foresight Link)
Bromwich, T. (EPSRC DTA)
Campbell, E. (QIP IRC)
Campbell, P.J.D. (CASE: BNFL)
Castro Diaz, L. (Regenesys / Linacre)
Chan, S.C. (EPSRC)
Chen, X. (self-supporting)
Chen, Y. (self-supporting and Linacre)
Clark, L. (EPSRC DTA / Hitachi)
Clarke, E. (EPSRC CASE: Corus)

Cosgriff, E. (Department)
Dancer, C. (EPSRC DTA)
Danvirutai, P. (Thai Gov.)
Dark, C.J. (EPSRC DTA)
Davidson, I. (CASE: Alcoa Extrusions)
Deak, D. (EPSRC)
Dudeck, K. (Clarendon)
Eggeman, A. (EPSRC DTA + CASE: Johnson Matthey)
Fitzsimons, J. (Helmore / EPSRC DTA)
Fraser. K. (EPSRC DTA)
Gauger, E. (EC QIPEST/DTA)
Ge, L. (Clarendon)
Gilbert, M. (UKAEA)
Grazioso, F. (EPSRC/HP)
Grennan-Heaven, N. (CASE: Oxford Nanoscience)
Guo, S. (K C Wong)
Habgood, M. (QIP IRC)
Haigh, S. (EPSRC DTA)
Hinchliffe, C. (CASE: Rolls-Royce)
Howells, D. (CASE: Dupont)
Islam, P. (Faraday CASE: Merck)
Jones, M. (EPSRC)
Jordan, D. (EPSRC DTA)
Joseph, T. (CASE: UKAEA)
Karney, G. (EPSRC DTA)
Kawata, K. (Toppan Printing Co.)
King, O. (EPSRC)
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Korsah, M. (EPSRC)
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Lui, A. (EPSRC DTA)
Marques, V. (EPSRC)_
Marsh, H. (EPSRC DTA)
Marshall, M. (self-supporting)
Martin, C. (EPSRC)
Mathieson, D. (OPSYS)
Morgan, D.L. (EPSRC)
Morley, A. (EPSRC DTA)
Morley, G. (EPSRC Foresight Link)
Morton, J. (EPSRC DTA / NEDO)
Mueller, M. (EPSRC DTA/Imago)
Mukhopadhyay, A. (Clarendon)
Murphy, J. (EPSRC/ St Hugh's College)
Newell, D. (CASE: Oxford Applied Research)
Nicholls, R. (EPSRC DTA, St Catherine's Scholarship)
Okayasu, T. (Oji Paper Co.)
Park, S-B. (self-supporting)
Pinitsoontorn, S. (Thai Gov.)
Plant, S. (EPSRC DTA)
Porcu, M. (EPSRC DTA / EU)
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Shaw, A. (EPSRC)
Sher, P-H. (self-supporting)
Shih, S-J. (self-supporting)
Shinotsuka, K. (self-supporting)
Shuo, H. (self-supporting)
Smart, K. (EPSRC)
Srimanosaowapak, S. (Thai Gov.)
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Stoll, A. (MoD)
Stowe, D.J. (EPSRC)
Suttle, H. (CASE: DuPont)
Tarleton, E. (EPSRC)
Thomas, G. (CASE: UKAEA)
Tiwari, A. (Clarendon)
Todorovic, M. (Scatchered Scholarship)
Tseng, Y-T. (self-supporting)
Tyrrell, E. (EPSRC DTA)
Vlandas, A. (EPSRC, St Cross College)
Wahl, D. (EPSRC)
Waller, J. (EPSRC)
Walpole, A. (EPSRC DTA)
Walton, R. (EPSRC DTA)
Wang, C. (EPSRC)
Wang, H. (Clarendon/ORS)
Waring, M. (EPSRC DTA)
Weber, K.U. (EPSRC)
Whyte, E. (CASE:Corus)
Womersley, H. (EPSRC)
Wu, C. (self-supporting)
Xie, Z. (Clarendon /ORS)
Xu, J. (self-supporting)
Xu, Q. (Dorothy Hodgkin)
Xu, S. (EPSRC)
Zandbergen, M. (Netherlands Inst. Mat. Research)
Zhang, J. (Clarendon, ORS, Queens College)
Zhang, K. (self-supporting)
Zhao, X. (self-supporting)
Zhou, Dr Z. (UKAEA)
Zhu, C. (Clarendon)
Zhu, M. (K.C.Wong / ORS)

*(Please note that student lists are correct at the time of going to press.)*

## Part II Students (4th Year Undergraduates)

Materials Science
Bent, M.
Britton, T.
Brooke-Hitching, M.
Copplestone, C.
Duffus, P.
Gregori, N.
Moore, K.
Ross, A.
Rounthwaite, N.
Singh, S.
Taylor, L.
Thomas, M.

Materials, Economics and Management
Chan, T.
Kay, A.D.
Mallam, E.J.
Mittermaier, M.M.H.
Ta, L-C.
Venugopal, S.

Engineering and Material Science
Armitage, P.

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Mrs. P. Topping
Mr. R.W. Turner
Mr. R. Vincent
Ms. L. Vockins
Mr. L. Walton
Mr. D. Williams

## Academic Visitors (1st Oct 2004 – 30th Sept 2005)

Ares Fernandez, Dr Jose, Department of Materials, University of Oxford, UK
Asanovic, A/Prof. Vanja, Faculty of Metallurgy & Technology, Serbia & Montenegro
Audebert, Dr Fernando, Buenos Aires University, Argentina
Balat, Dr Jelena, University of Belgrade, Serbia & Montenegro
Balazs, Prof. Anna, University of Pittsburgh, USA
Bhatti, Dr Rashid, Qinetiq, UK
Birou, Mr Thierry, CEMES/CNRS, Toulouse, France
Bishop, Dr Hugh, MIMIV Limited, Abingdon, UK
Bucknall, Dr David, Georgia Institute of Technology, Atlanta, USA
Burgmann, Dr Flame, RMIT University, Melbourne, Australia
Butler, Dr Paul, Crown cork & Seal Co. Inc., Wantage, UK
Chauke, Mr Richard, University of the North, Sovenga, South Africa
Chen, Prof. Xiaohua, Hunan University, China
Choi, Dr Si-Young, Korea Advanced Institute of Science & Technology, Korea
Creatore, Dr Mariadriana, Eindhoven University of Technology, The Netherlands
Doyle, Dr Tony, Doyle & Tratt Products Ltd, Horsham, UK
Dudarev, Dr Sergei, Culham Science Centre, UK
English, Dr Colin, BNFL, Didcot, UK
Eyre, Prof. Brian, CLRC, Rutherford Appleton Laboratory (retired Chair), UK
Fairchild, Mr John, Forensic Alliance Ltd, Culham Science Centre, UK
Falster, Dr Bob, MEMC, Begbroke, UK
Findlay, Dr Scott, University of Melbourne, Victoria, Australia
Flewitt, Dr Peter, BNFL & Bristol University, UK
Gabrys, Dr Barbara, Department of Continuing Education, University of Oxford, UK
Han, Prof. Zhiwu, Jilin University, Changchun, China
Haseeb, Mr Abdul, Bangladesh University of Engineering & Technology (BUET), Bangladesh
Jadoon, Dr Ammer, AWE, Aldermaston, Berks., UK
Jefferson, Prof. John, QinetiQ, UK
Khlobystov, Dr Andrei, University of Nottingham, UK
Kiselev, Prof. Nikolai, Russian Academy of Sciences, Moscow, Russia
Kou, Prof. Shengzhong, Lanzhou University of Technology, China
Kruska, Ms Karen, TU Clausthal, Germany
Larson, Dr David, Seagate Technology, USA
Matijasevic, Ms Milena, SCK-CEN, Mol, Belgium
Mitzutani, Prof. Uichiro, Toyota Physical & Chemical Research Institute, Japan
Muhl, Dr Thomas, Leibniz Institute, Dresden, Germany
Myhra, Dr Sverre, Griffith University, Australia
Nguyen-Manh, Dr Duc, Culham Science Centre, UK
Norenberg, Dr Christiane, Swansea University, UK
Ogura, Mr Tomo, Tokyo Institute of Technology, Japan
Paganin, Dr David, Monash University, Victoria, Australia
Palmer, Dr Ian, [Private Researcher], UK
Park, Prof. Myung-Beom, Korea Third Military Academy, Korea
Pethica, Prof. John, Trinity College, Dublin, Ireland
Poullain, Prof. Giles, University of Caen, France
Pusztai, Dr Laszlo, Hungarian Academy of Sciences. Budapest, Hungary

Reid, Prof. Michael, Canterbury, New Zealand
Ruterana, Dr Pierre, SIFCOM, France
Sachlos, Mr Terry, Begbroke Directorate, UK
Sanchez Fuentes, Dr Ana, University of Cadiz, Spain
Schönberger, Dr Uwe, Max-Planck Institute, Stuttgart, Germany
Sloan, Dr Jeremy, University of Surrey, UK
Smith, Dr Peter, GCHQ, UK
Stoneham, Prof. Marshall, University College London, UK
Tanaka, Dr Yasuhiro, Kagawa University, Japan
Titchmarsh, Prof. John, Department of Materials, University of Oxford (retired), UK
Tohmori, Mr Masashi, University of Shiga Prefecture, Japan
Veseley, Dr Drahosh, OCAMAC Fellow, UK
Visart de Bocarmé, Dr Thierry, Free University Brussels, Belgium
Wang, Prof. Zhiping, Lanzhou University of Technology, China
Warren, Dr Paul D, Pilkington plc, UK
Whitehouse, Prof. Colin, CCLRC Daresbury Laboratory, UK
Wood, Prof. John, CCLRC Rutherford Appleton Laboratory, UK
Wu, Dr Houzheng, Coventry University, UK
Yang, Dr Judith, University of Pittsburgh, USA
Zhao, Dr Kunyu, Kunming University of Science & Technology, China
Zhou, Dr Zhongfu, University of Cardiff, UK

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Mr. D.K. McLachlan, formerly Tax partner Price Waterhouse Coopers
Dr. K.A.Q. O'Reilly, Department of Materials, University of Oxford
Mr. C.G. Purnell, formerly Technical Director, Brico Engineering
Miss L. Scruby, trainee teacher
Professor G.D.W. Smith, FRS, Department of Materials, University of Oxford
Mr. R. Strawson, Head of Physics, Abingdon School

## Industrial Advisory Panel

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Much of the research in the department is supported by grants from Research Councils, industrial companies, government departments, overseas governments, trusts and charitable foundations, learned societies and city livery companies. The department is greatly indebted to these organisations for their generous support.

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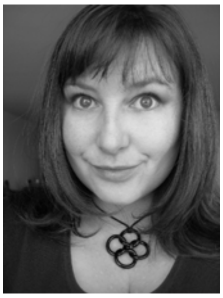
SEEDA
Southampton University
Thai Government
The Royal Society
Toppan Printing Company
Trackdale
TTI Process Technology Center
UKAEA
Wellcome Trust

# Profiles of Academic Staff

**Dr. Hazel Assender** **Lecturer in Materials**
*Linacre College*

Research, both experimental and modelling, on a range of polymer and polymer composite materials. Particular areas of interest include the relationship between processing and microstructure, surface characterisation and modification, polymer photovoltaic materials and polymer coatings and thin films, in particular vacuum roll-to-roll deposition of coatings on to polymer substrates.



**Dr. Amanda Barnard** **Glasstone Fellow**
*The Queen's College*

Fundamental studies of the shape of nanomaterials (nano-morphology), and how it affects nanoscale phase transitions and phase co-existence. Using primarily thermodynamic theory and ab initio computer simulations, current projects include the development of a general, multi-scale theory of nano-morphology dependent upon experimentally relevant factors such as size, composition, temperature, defects and surface chemistry. Secondary interests include investigations of how shape affects the stability of doped and undoped carbon nanomaterials, such as nanodiamond, diamond nanowires and hybrid nanocarbons.

**Dr. Simon Benjamin** **Royal Society University Research Fellow**
*Exeter College*

Physics of computation. Design and realization of architectures for new forms of information processing, especially quantum computing. Theoretical work relating to the design, growth and characterization of solid state nanostructures for computation, with particular current emphasis on (a) quantum dots systems, both self assembled and lithographically defined, and (b) fullerene systems (nanotubes, endohedral C60, etc.) Secondary interest in other areas of quantum information theory, such as quantum game theory.

**Dr. Catherine Bishop** **Career Development Fellow**
*St Anne's College*

Phase-field modelling of materials to predict transitions in interfacial structure. The relationship between continuum and atomistic descriptions of materials.

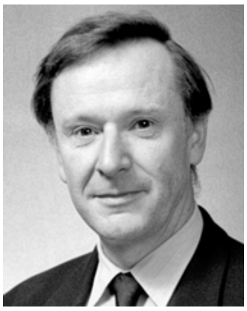
**Dr. Roger Booker** **Emeritus Reader in Electronic Materials**
*Wolfson College* **OCAMAC Senior Fellow**

Microscopic studies of semiconductor materials and devices and the effects of structures on properties.

**Professor Andrew Briggs** — **Professor of Nanomaterials**
*Wolfson College* — **Director of the Quantum Information Processing IRC**

Director of Quantum Information Processing Interdisciplinary Research Collaboration.

- Holliday Prize, Institute of Materials, 1984
- Metrology award for World Class Manufacturing, 1999
- Honorary Fellow of Royal Microscopical Society, 2000



**Professor Sir Richard Brook OBE FREng** — **Emeritus Professor**
*St Cross College*

Processing and properties of ceramic materials.

[ Currently Director of the Leverhulme Trust]

**Dr. Martin Castell CPhys** — **Lecturer in Materials**
*Wolfson College*

Elevated temperature scanning tunnelling microscopy of oxide surfaces to identify atomic scale defects relevant to catalytic processes and nanotechnology. Investigation of patterned oxide surfaces for use as templates in nanoelectronics. High resolution secondary electron imaging in the SEM of semiconductor nanostructures and devices to study local strain, dopant distributions, dopant diffusion and deactivation.

**Professor Alfred Cerezo** — **Professor of Materials**
*Wolfson College*

Investigations of solid state phase transformations on the atomic scale by a combination of high resolution microscopy and computer modelling. Development of atom probe microanalysis and its application to a range of materials.

- E.W.Müller Outstanding Young Scientist Award, Int. Field Emission Soc. 1988
- C.R. Burch Prize, British Vacuum Council, 1990
- Sir George Beilby Medal and Prize, 2001
- NPL National Award for Innovation in Measurement 2004

**Professor David Cockayne FRS, FInstP, FAInstP** — **Professor in the Physical Examination of Materials**
*Linacre College*

Development of electron optical techniques for investigating structure of materials; defects in crystalline material; structure of amorphous materials; refinement of structures including quantum dots and interfaces ; remote microscopy.

- President of the International Federation of Societies of Microscopy, 2003-7.

**Dr. Alison Crossley** — **Senior Research Fellow**

The application of surface science to a wide variety of materials. Materials problem solving for industry.

**Dr. Jan Czernuszka** **Lecturer in Materials**
*Trinity College*

Interaction of biochemicals with ceramics. Formation of nanolaminates, composites and coatings at room temperature. Development of novel bone analogues, drug delivery systems and hierachically controlled structures. Mechanical properties of natural materials. Tissue engineering of scaffolds.

- CBI / Toshiba Year of Invention, winner of University section, 1993

**Dr. Ralf Drautz** **MML Research Fellow**
*Wolfson College*

Theory of effective interatomic interactions. Application to understanding, predicting and designing properties of materials.

- Otto Hahn Medal and prize 2003

**Professor Colin English FREng** **Visiting Professor**

Research interests are focussed on understanding of the mechanisms controlling the degradation of reactor structural components. This necessitates developing an understanding of processes occurring at the atomic scale, as frequently, there is a direct link between mechanisms occurring on this scale and the macroscopic performance of reactor plant components. The primary areas of interest are: Reactor Pressure Vessel embrittlement, environmentally assisted corrosion in reactor core components, irradiation and thermal ageing effects in Zr alloys employed in nuclear applications, and irradiation effects in reactor graphite.

**Professor Brian Eyre FRS FREng** **Senior Visiting Fellow**

Main areas of interest are electron microscopy studies of irradiation damage in metals and alloys and studies of the deformation and fracture processes of metals and alloys.

**Dr. Marina Galano** **Career Development Fellow**
*St Edmund Hall*

Manufacture and characterisation of nanostructured lightweight alloys, in particular Al based alloys. Study of the microstructure and phase transformation processes of rapid solidified alloys, mechanical properties and their relationship with the microstructure.

- Hetherington Prize 2003
- Niobium Student Research Award 2004

**Professor Patrick Grant** **Cookson Professor of Materials**
*St Catherine's College* **Director of Faraday Advance**

Advanced processing of materials, such as spray forming of metals, composites and coatings. Research has focused on the relationship between heat and mass flows and microstructures. On-line monitoring and numerical simulations are used to help understand the underlying process physics.

**Dr. Nicole Grobert** — **Royal Society Dorothy Hodgkin Fellow**
*Wolfson College*

Production of carbon nanotubes and modified carbon nanotubes by chemical vapour techniques. In-situ investigation and characterisation of nanotube growth in order to elucidate important parameters for the controlled formation of carbon nanotubes and related materials.

- Pergamon Prize 2001

**Professor Chris Grovenor** — **Professor of Materials**
*St Anne's College* — **Head of Department**

Applied superconductivity and the processing of electronic materials, and leader of the group developing applications for our new CAMAC NANOSIMS 50.. Other recent work has focused on understanding the fundamental limitations in the processing of high temperature superconducting materials and developing techniques for reliable preparation of HTS components.  The deposition and characterisation of nano-structured oxide films for gas permeation and photovoltaic electrode applications has been a growing area of interest.

**Professor Sir Peter Hirsch   FRS, Hon. FIMMM** — **Emeritus Professor**
*St Edmund Hall*

Electron microscopy of defects in crystals and modelling mechanical properties of crystalline materials in terms of dislocation processes.

- Royal Society : Hughes Medal 1973 and Royal Medal, 1977.
- Metals Society Platinum Medal 1976
- Wolf Prize in Physics, 1983
- Acta Metallurgica Gold Medal, 1997
- Foreign Associate of the US National Academy of Engineering 2001
- Foreign Honorary Member of American Academy of Arts and Sciences 2005
- Lomonosov Gold Medal of Russian Academy of Sciences 2005

**Professor John Hunt FRS** — **Emeritus Professor**
*St Edmund Hall*

Modelling and understanding fundamental solidification processes: This has included work on eutectics, peritectics, cellular and dendritic growth. The fundamental understanding has been applied to casting processes. Recent work includes experimental and theoretical studies of twin-roll casting and differential scanning calorimetry.

- The Royal Society Armourers and Brazier's Award, 2001.
- The Bruce Chalmers Award, TMS AIME, 1996.
- Rosenhain Medal and Prize, Institute of Materials, 1981.
- C.H. Mathewson Gold Medal, TMS AIME,, 1967.

**Dr. John Hutchison** — **Reader in Materials**
*Wolfson College*

Development of high resolution electron microscopy for structural characterisation of new materials including :  quantum dots, inorganic fullerenes and complex oxides. Development of controlled environment electron microscopy for in-situ study of catalysts and of gas-solid reactions. Development and applications of aberration-corrected HREM.

- Glauert Medal, Royal Microscopical Society, 1975
- President, Royal Microscopical Society, 2002

**Dr. Mike Jenkins** — **Reader in Materials**
*Trinity College* — **Director of Electron Microscope Facilities**

Radiation damage, transmission electron microscopy, phase stability under irradiation, stress corrosion cracking, intermetallics. Recent work has focused on fundamental mechanisms of radiation damage, especially displacement cascade processes, mechanisms of embrittlement of pressure vessel steels, radiation damage in materials for future fusion reactors and new methods for characterizing small defect clusters.

**Dr. Colin Johnston** **Senior Research Fellow**

Materials for harsh environments including aerospace and transport materials. High temperature electronics including packaging and reliability. Failure analysis and design for inherently reliable operation at elevated temperatures.

**Professor Angus Kirkland** **Professor of Materials**
*Linacre College*

Ultra High Resolution Transmission Electron Microscopy. Image Simulation and Processing. The investigation of new approaches to quantitative microscopy (theory and experiment). Structural studies of nanocrystals, inorganic oxides and surfaces. The development of new detectors for imaging with high energy electrons. Remote control of electron optical instruments.

**Dr. Ahmit Kohn** **RAE/EPSRC Research Fellow**

Correlating magnetic properties to microstructure in thin magnetic films using high-resolution,analytical and Lorentz transmission electron microscopy.

**Dr. Brendon Lovett** **Royal Society University Research Fellow**

Design and realization of architectures for new forms of information processing, especially quantum computing. Theoretical work relating to the design and characterization of solid state nanostructures for computation, with particular current emphasis on (a) quantum dots systems (b) fullerene systems (nanotubes, endohedral C60, etc.) (c) defects in diamond. In particular, I do calculations of how to control and manipulate interactions between nanostructures such that entangled states might be produced between them. I also work on understanding the nature of quantum decoherence in solid state systems. Further interests include entanglement in more exotic many-body states, particularly the Kondo singlet.

**Dr. John Martin Sc. D, C. Eng., FIMMM** **Emeritus Reader**
*St Catherine's College* **OCAMAC Senior Fellow**

The relationship between the structure and the properties of metallic materials, particularly precipitation hardening, recrystallization and grain growth, fatigue and fracture.

- Sidney Gilchrist Thomas Medal and Prize, Institute of Materials, 1986.
- Platinum Medal, Institute of Materials, 2001.

**Dr. Peter Nellist** **Lecturer in Materials**
*Corpus Christi College*

Application and development of high-resolution scanning transmission electron microscope techniques (STEM). Atomic resolution Z-contrast imaging. Electron energy-loss spectroscopy. Applications of spherical aberration correctors. Development of three-dimensional imaging and analysis techniques using optical depth sectioning and confocal techniques. Structural determination of inorganic nanowire materials.

**Dr. Peter Northover** **Senior Research Fellow**
*St Catherine's College / St Cross College*

Non-ferrous and precious metallurgy and metalwork in ancient and historical contexts and their experimental reproduction; engineering metallurgy of the industrial revolution; coinage technology; long-term stability of the microstructure; interaction of buried metal with the environment.

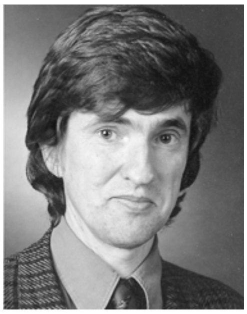
**Dr. Keyna O'Reilly** **Lecturer in Materials**
*The Queen's College*

Solidification processing of advanced materials from laboratory scale simulations through to pilot scale processing plant, with particular interests in grain refinement and intermetallic phase selection. Also thermal analysis of phase transformations. Covering a wide range of materials including Al alloys, intermetallics, biomaterials, and solder alloys.

**Professor John Pethica FRS** **Visiting Professor**
*St Cross College*

Surface and nanometer scale properties of materials. Study of mechanical properties using nanoindentation and of surface atomic structure and transport processes using scanning tunnelling microscopy. Development of atom resolved AFM and force spectroscopy of single bonds.

- Holweck Medal, Société Francaise de Physique & IoP, 2002.
- Hughes Medal, The Royal Society, 2001.
- Rosenhain Medal, Institute of Materials, 1997.
- Sabbatical Chair, Sony corporation R&D, Japan, 1993-4.



**Professor David Pettifor FRS** **Isaac Wolfson Professor of Metallurgy**
*St Edmund Hall* **Director of Materials Modelling Laboratory**

Development and application of electron theory to understanding and predicting the properties of materials, in particular metals, alloys and covalently bonded semiconductors and ceramics.

- Royal Society Armourers and Brasiers' Medal 1999
- William Hume-Rothery Award, TMS 1995.
- Hume Rothery Prize, Institute of Materials, 1990.

**Professor Steve Roberts** **Professor of Materials**
*St Edmund Hall*

Mechanical behaviour of materials, especially their response to surface deformation and the brittle-ductile transition. Materials for fusion power plants. Micromechanical testing. Studies aim at linking modelling at the defect and dislocation level with experimental studies of well-characterised materials.

**Professor George Smith FRS** **Professor of Materials**
*Trinity College*

Phase transformations, atom probe analysis. Studies of the role of alloy elements and trace additions on the microstructure, heat treatment and properties of steels and non-ferrous alloys. Atomic scale studies of heterogeneous catalysts.

- Acta Materialia Gold Medal 2005
- NPL National Award for Innovation in Measurement 2004
- Rosenhain Medal and Prize, 1991
- Sir George Beilby Medal and Prize, 1985

**Dr. Jason Smith** **Lecturer in Materials**
*Mansfield College*

Leader of the Photonic Nanomaterials Group in which research is focused on optical and electronic properties of solid state nanostructures for applications such as optoelectronics devices, quantum information processing and photovoltaics. At present the Group's research involves two such systems - semiconductor nanocrystals and nitrogen-vacancy defects in diamond (see project descriptions below) - which we investigate using luminescence-based optical techniques..

**Dr. Susannah Speller** **RAE/EPSRC Research Fellow**

Processing of High Temperature Superconducting thin films on flat and curved substrates for a range of device applications. Recent work has focused on grain boundary properties and texture development in Tl-based HTS films. A growing area of interest is the development of superconducting meta-materials for novel applications such as near field NMR microscopy.

**Dr. John Sykes** **Reader in Materials**
*Mansfield College*

Corrosion of metals. Conversion treatments, protection by organic coatings, studies of coating breakdown. Passivity, chloride-induced pitting, corrosion of steel in concrete, metal hydrides for energy storage.

**Professor John Titchmarsh** **Senior Visiting Research Fellow**
*St Anne's College*

Techniques for electron microscopy materials analysis: electron energy loss spectroscopy and X-ray analysis. Mechanical properties, precipitation and segregation in nuclear reactor alloys, ferritic steels, surface engineered hard coatings and ceramic composites. Extraction of information using chemometric techniques.

**Dr. Richard Todd** **Lecturer in Materials**
*St Catherine's College* **Director of Oxford Centre for Advanced Materials and Composites**

Mechanical properties of ceramics and metals. Most research revolves around oxide cerar microstress measurements and superplastic metals. Current interests include the processing properties of ceramic nanocomposites (including functional nanocomposites based on $BaTiO_3$), either particulate or carbon nanotube reinforcements, high spatial resolution (~100nm) measuren of stresses in metals and ceramics, and high spatial resolution surface studies of superplastic flov

- Pfeil Award, Institute of Materials, 2001.

**Dr. Drahosh Vesely** **OCAMAC Senior Fellow**
*Wolfson College*

Light and electron microscopy, electron beam damage and spectroscopy are used to s crystallographic morphology of spherulitic structures, nucleation and crystallization, stabiliza degradation, electrical conductivity, fluorescence, diffusion, permeability, solubility and mecha properties of polymeric compounds.

**Professor Mike Whelan FRS** **Emeritus Professor**
*Linacre College*

Transmission electron microscopy of materials, transmission electron diffraction of thin specimens (theory and application to crystal lattice defect observation). Reflection electron diffraction of surfaces (theory and applications to molecular beam epitaxial growth).

- Distinguished Scientist Award, Microscope Society of America, 1998
- Hughes Medal, Royal Society, 1988
- C.V. Boyes Prize, Institute of Physics, 1965

**Dr. Angus Wilkinson** **Lecturer in Materials**
*Corpus Christi College*

Mechanics at the microscopic scale, both experimental and modelling. Dislocation modelling of fatigue and fracture processes. Development of SEM based diffraction methods (ECCI and EBSD) for imaging lattice defect distributions and measuring local internal strain distributions.

**Dr. Peter Wilshaw** **Reader in Materials**
*St Anne's College*

Characterisation of the electrical and mechanical properties of defects in semiconductors. The development of silicon substrates with improved properties. High resolution 2D mapping of dopant distributions in semiconductors. Development of a bioactive coating for metal implant prostheses.

**Professor Colin Whitehouse** **Visiting Professor**

Council for the Central Laboratories of the Research Councils (Rutherford-Appleton and Daresbury Laboratories).

**Professor John Wood FREng** **Visiting Professor**
**Wolfson College Industrial Fellow**

Chief Executive, Council for the Central Laboratories of the Research Councils (Rutherford-Appleton and Daresbury Laboratories). Materials processing, biomaterials, surface engineering, Materials Foresight, Strategic policy for large facility research.

[Professor of Materials Engineering, University of Nottingham (on secondment)]

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# A. Structure and Mechanical Properties of Metals

## Fundamentals of cyclic deformation and fatigue crack initiation

*Dr. A.J. Wilkinson, Dr. S.G. Roberts*

The evolution of dislocation microstructures produced during cyclic deformation is being examined using electron channelling contrast imaging, a novel SEM technique. The objective is to understand the reasons for dislocation patterning and subsequent strain localisation leading to the initiation and early growth of fatigue cracks.

## Strain Tensor Mapping at the Nanoscale using EBSD

*Dr. A.J. Wilkinson*

A technique for probing local elastic strain fields using electron back scatter diffraction patterns has been developed. The technique combines a spatial resolution of ~20 nm with a strain sensitivity of 2 parts in 10000. It is being used in conjunction with electron channelling contrast imaging to characterise local strain and defect distributions in semiconductor materials and devices. Materials systems being studied include SiGe/Si, epitaxially laterally overgrown GaN films, device isolation structures, and crack tips.

## Fatigue Crack Initiation in Polycrystals

*P. Littlewood, Dr. M. Nardone*, Dr. A.J. Wilkinson, Dr. F.P.E. Dunne*, Dr. S.G. Roberts, Professor D.A. Hills**

We aim to carry out fundamental experimental and computational studies on fatigue crack initiation to understand where, why and how cracks initiate under conditions of low and high cycle fatigue. Experimental work is to include the use of 2D directionally solidified Ni superalloy material in which the development of slip bands under cyclic loading will be investigated and quantified in characterised microstructures (obtained using SEM with EBSD). Effects of different grain boundary character on crack nucleation behaviour in Ti alloys with different micro-textures will also be studied. Experimental results will be compared to polycrystal plasticity simulations. (*Engineering Science)

## Fundamentals of brittle-ductile transitions

*Dr. S.G. Roberts, Professor Sir Peter Hirsch, Dr. A.J. Wilkinson*

Cleavage failiure in the Brittle-transition of steels is being treated in terms of a model in which the cleavage is initiated at a microcrack situated in the stress field ahead of a macroscopic crack. The plastic zone around the microcrack is modelled by computer simulations of dislocation arrays around the micro-crack-tips. Dislocation shielding plays an important part in determining the fracture stress. The model predicts a fracture stress independent of yield stress, in accord with experiments. (Funded by EPSRC, AEAT and HSE)

## TEM investigation of stress corrosion cracking in Inconel 600

*Dr. S. Lozano-Perez, Professor J.M. Titchmarsh, Dr. M.L. Jenkins, Dr. K. Fujii**

Intergranular stress corrosion cracking in Inconel 600 in the heat exchangers and other components in the primary circuit of PWR power generating plant is an important safety issue. The project will develop techniques for TEM specimen preparation using FIB to allow investigation of the nucleation and growth of SCC. Characterisation of precipitation and segregation at boundaries will enable key microstructural factors to be identified that contribute to SCC. (Funded by INSS* and EPSRC)

## Multi-scale modelling and simulations of cleavage fracture in steels

*Professor S.J. Chapman*, Dr. S.G. Roberts, Dr. J.R. Ockendon*, Dr. A.J. Wilkinson, Dr. R. Voskoboynikov, A. Kumar*

The project aims to formulate continuum models of plastic flow in three dimensions, and to apply these to crack initiation and propagation in multi-phase materials. The modelling is being carried out in parallel with experimental studies of fracture nucleation and crack-tip plastic zones in steels with simplified microstructures. (*Oxford Centre for Industrial and Applied Mathematics) (Funded by EPSRC)

### *Brittle-ductile transitions in BCC metals for fusion power applications*

*Dr. A. Giannattasio, T.D. Joseph, Dr. S.G. Roberts, Dr. A.J. Wilkinson, Dr. S.L. Dudarev**

The project investigates the brittle-to-ductile transition in vanadium, tungsten and iron-chromium alloys up to 12%Cr (all these metals are the basis for proposed fusion power plant alloys). Pre-cracked miniature bend specimens of single crystals and polycrystalline materials are fracture tested in the temperature range 77 - 450K. The effect of dislocation motion around the crack tips on fracture stress is examined, and modelled using dynamic-dislocation simulations. (*UKAEA Culham) (Funded by EPSRC, UKAEA, EU)

### *Core structure of screw dislocations in BCC metals*

*Professor Sir Peter Hirsch*

Isotropic elasticity calculations show that the symmetrical 3-fold dissociation of screw dislocations in b.c.c. metals is unstable. Yet atomistic computer calculations usually show 3-fold dissociated structures, dissociated mainly on {110} planes. It turns out that using anisotropic elasticity the symmetrical 3-fold dissociation of {110} is stable or metastable. A possible 6-fold dissociation will be investigated.

### *Investigation of grain growth during fabrication of ferritic steel rod*

*S. Ahmed, Professor J.M. Titchmarsh*

This project investigate the relationship between microstructural variations and mechanical properties of ferritic steel rod, in particular, variations in grain size will be correlation with segregation of low atomic number elements (B, N, C) using microanalytic techniques such as NanoSIMS, TEM, micro-diffraction etc. (Funded by Corus and EPSRC) (In collaboration with Corus)

### *Micromechanical testing*

*D. Armstrong, Dr. S.G. Roberts, Dr. A.J. Wilkinson*

The project will develop new methods of testing mechanical properties at the micron scale, using a combination of focussed ion beam machining (to produce specimens) and atomic force microscopy / nanoindentation (to test them). The methods will be applied to testing thin films, ion-irradiated layers, interfaces and properties of individual grains and grain boundaries in alloys.

### *Surface effects in superplastic deformation*

*M.A. Rust, Dr. R.I. Todd*

The superplastic deformation of aluminium and Sn-Pb alloys is being studied with particular reference to surface observations. FIB is being used to etch submicron reference grids on the surface and EBSD is being used to characterise grain boundaries of interest. Aspects being studied include the origin of surface ridges and other inhomogeneous aspects of flow, co-operative grain boundary sliding, intragranular deformation and the nature of grain boundaries. (In collaboration with Superform Metals)

### *Internal stresses and stored energy in steels*

*E. Clarke, Dr. A.J. Wilkinson, Dr. R.I. Todd, Dr. D. Crowther*, Dr. A. Howe**

Several methods of measuring microstresses in steels are being investigated, with a view to developing a robust method of measurement. The main methods to be tried are (i) XRD line profile analysis, (ii) EBSD, and (iii) nanoindentation. The microstresses are thought to be important in many steels, and link processing to properties in much the same way as microstructural features such as grain size. (In collaboration with *CORUS and with support from EPSRC and CORUS)

### *A nanoindentation study of slip transmission at grain boundaries*

*T.B. Britton, Dr. A.J. Wilkinson*

Nano-indention produces very localized plastic deformation. If the indenter is near a grain boundary then slip will initially be blocked, but under continued loading transmission of slip to the neighbouring grain will occur. We will use the nanoindenter, AFM, SEM and electron back scatter diffraction to study conditions under which slip transmission occurs at boundaries of different character in representative bcc, fcc and hcp metals. Indents will be made at different distances from selected grain boundaries. SEM and AFM will be used to examine surface topography for evidence of slip transfer to the neighbouring grain. EBSD will be used to characterise the grain boundary geometry, and to map local strain and lattice curvature distributions near the indents. We hope to correlate resistance to slip transmission with grain boundary geometry.

## *Electron back scatter diffraction studies of cold deformation in stainless steels and nickel alloys*

*Dr. M. Kamaya*, Professor J.M. Titchmarsh, Dr. A.J. Wilkinson*

We are using electron backscatter diffraction to measure the plastic strain present in stainless steel and nickel alloys following tensile loading. We quantify the spread of the crystal orientation within individual grains arising due to dislocation accumulation and correlate this with imposed plastic strain. We are developing parameters that have good correlation with the degree of the plastic strain and are independent of the measurement conditions such as the number of data and step size in the crystal orientation map, electron beam condition, grain size and material. We hope to apply the method to measurement of cold work in nuclear power plant components. (*Institute of Nuclear Safety Systems, Japan)

## *Mechanical analysis of environmentally assisted cracks*

*A. Stoll, Dr. A.J. Wilkinson*

This project will develop both computer simulation and experimental methods for studying the local distributions of stress and strain near inter-granular stress corrosion cracks (IGSCC). The multiply deflected and branched crack paths that are typical in IGSCC lead to extensive crack-crack interactions and cause significant, complicated variations in the local driving force for crack advancement (K) and hence similar complexity in crack growth rates. The studies will centre on modified 304 and 316 stainless steels. Dislocation mechanics methods will be used to simulate the development of stress fields and plastic zones associated with IGSCC as they grow through different simulated microstructures. Experimental validation of the computer models will be undertaken using SEM based diffraction methods. In particular advantage will be taken of our recent advance in development of EBSD elastic strain mapping techniques. This project is part of a much wider programme of research on 'Multi-scale approaches to enhance materials performance: Environmentally-assisted degradation' funded by the MoD through the Nuclear Propulsion Critical Technology scheme. Project partners are the Universities of Manchester and Birmingham, and Johnson-Matthey Technology Centre.

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# B. Non-Metallic Materials

## I - CERAMICS AND COMPOSITES

### Oxide Nanocomposites

*A. Mukhopadhyay, Dr. R.I. Todd*

Work in Oxford has shown that alumina/SiC nanocomposites offer enormous improvements in resistance to severe wear compared with pure alumina. Commercial takeup of these materials has been limited, however, owing to the requirement to sinter these materials in inert gas in order to prevent oxidation of the SiC. Routes for producing 100% oxide nanocomposites are being explored that will avoid this problem.

### Plasticity in oxide nanocomposites

*A. Mukhopadhyay, Dr. R.I. Todd*

Alumina/SiC nanocomposites exhibit much more surface plasticity and much less brittle fracture than pure alumina when subjected to severe grinding. This project is investigating the extent to which this also applies to bulk deformation of alumina and MgO based nanocomposites.

### Perovskite-based ceramic nanocomposites

*A. Ross, H. Wang, Dr. H. Zheng, Dr. R.I. Todd*

Functional ceramics based on perovskite structures have many interesting and useful properties (e.g. they can be piezo- and pyro-electric). Much research has gone into tailoring their properties to particular applications by changing their composition, but relatively little work has been done on changing their properties by the addition of second ceramic phases. Recent work in Oxford has shown that very small volume fractions (e.g. 1-2%) of nanophase additions can have dramatic effects on the properties of structural ceramics, and research elsewhere gives reason to believe that this might also be the case with functional ceramics. Furthermore, some of these effects might be synergistic in that they could improve both the mechanical and the functional properties of the material. The aim of the project is to explore the interaction between internal stresses, ferroelectric domain structure and functional and mechanical properties of such nanocomposites, starting with the barium titanate/SiC system. (In collaboration with Morgan Electro Ceramics)

### Wear and indentation of alumina/SiC nanocomposites

*A. Limpichaipanit, Dr. S.G. Roberts, Dr. R.I. Todd*

The wear and indentation of alumina/SiC nanocomposites are being investigated with a view to explaining the reduction in size of surface pullouts and increased resistance to microcrack nucleation observed in extensive previous work in this Department. (With support from the Thai Government)

### Measurement and mapping of stresses in alumina with submicron resolution using cathodoluminescence in the SEM.

*Dr. R.I. Todd, Dr. P.R. Wilshaw, Dr. S. Galloway**

Stress measurement in alumina and other oxides using the shift of Cr3+ fluorescence peaks is well established, and is most often accomplished by stimulating the fluorescence using laser light focused on the specimen through an optical microscope. The stress can be measured with a spatial resolution down to several micrometers by this means. The same fluorescence lines can be stimulated by incident electrons, and we are investigating the possibility of making stress measurements with submicron resolution using the Cr3+ cathodoluminescence given off by Cr-doped alumina in the electron beam of an SEM. (* Gatan Ltd.)

### Surface mechanical properties of alumina-based materials

*S. Guo, Dr. R.I. Todd*

The project aims to develop a better understanding of the nature and origin of surface damage in ceramics based on alumina. The residual stresses caused by indentations, single scratches and standard grinding and polishing operations are being mapped using ruby R-line piezospectroscopy. High spatial resolution is being achieved by stimulating this fluorescence using light in conjunction with an optical microscope and electrons in the SEM (cathodoluminescence). The stress measurements are being correlated with direct SEM observations of cracking in sectioned specimens.

### *PLZT microstructures for high strain piezoelectric applications*

*M. Waring, Dr. R.I. Todd, Dr. L.P. Walker*, Dr K.S. Knight**

PLZT compositions close to the tetragonal/rhombohedral phase boundary are known to produce an exceptionally large strain for a given applied electric field. There are three contributions to the strain, namely electrostriction, the converse piezoelectric effect, and a field induced phase change. We are using electro-mechanical testing, Raman and electron microscopy and XRD to develop an improved understanding of these effects through a thorough study of the relationship between microstructure, and the grain size in particular, and properties. (*QinetiQ)(Supported by EPSRC)

### *Processing of nanograined alumina*

*M. Brooke-Hitching, Dr. R.I. Todd*

There are several papers in the literature about various aspects of powder processing of submicron alumina. These have shown some success but few if any of the papers have used all the ideas in the literature at the same time. This project aims to produce an optimised processing route that considers both the production of green bodies by wet shaping methods and the details of the sintering cycle to ascertain how far this combined approach can reduce the sintered grain size.

## II - BIOMEDICAL MATERIALS

### *Properties of biocomposites*

*Dr. J.T. Czernuszka*

Composites of natural polymers and sparingly soluble solids based on natural systems are being made and their microstructures and architectures together with their properties are being determined. New models of how this class of materials behave are being formulated.

### *Macro-assembled spheres of apatite*

*Q. Xu, Dr. J.T. Czernuszka*

Lipid spheres are being coated with apatite and then deposited on to metallic surfaces. We have achieved hierarchical control of the architecture of the macro-assembly on 5 length scales. The liposomes are being filled with biopharmaceutical agents.(Funded by Dorothy Hodgkins Scholarship, EPSRC)

### *Tissue Engineering and three-dimensional scaffolds*

*Dr. J.T. Czernuszka, Dr. E. Sachlos*, D.Wahl, Dr. C. Liu, Y-T. Tseng, R. Walton*

Three dimensional scaffolds are being developed for several major tissue engineering applications. There are extensive collaborations with research groups nationally and internationally and we are using tissue engineering to prepare bone, cartilage, arteries, heart muscles, heart valves and liver. (*Harvard, USA)

### *Three Dimensional Scaffolds for Tissue Engineering*

*D. Wahl, Dr. J.T. Czernuszka, Professor Z.F. Cui**, Professor B. Derby***, N. Reis***, Dr. C. Liu*

Scaffolds are being fabricated using novel ink jet printing techniques. The printing design and processing capabilities are being assessed and tailored to produce highly specified constructs. The mesostructure is being tailored to encourage vascularisation and subsequent tissue incorporation. The nanostructure, microstructure and mesostructure are all being tailored to optimise the degradation rate and mechanical properties. (Dept. Engineering Science, University of Oxford; ***Manchester Materials Science Centre) (Funded by EPSRC, DTI and the Wellcome Trust)

### *Tissue Engineering of Heart Valves*

*Dr. J.T. Czernuszka, Professor Sir Magdi Yacoub*, Dr. P. Taylor*, Dr. A. Chester*, S. Dreger*, Dr CT Bowles**, Y-T. Tseng*

Scaffolds for the tissue engineering of heart valves are being fabricated using the novel fabrication route developed in our laboratory. The scaffolds comprise collagen, elastin and pores, and these are arranged in a specific an sytematic manner to encourage the differentiation of mesenchymal stem cells. The performance of the scaffolds is monitored through changes in cell phenotype, tissue regeneration and mechanical property changes. The influence of bioreactor perfomance is being monitored. (*Heart Science Centre, Harefield Hospital, **Imperial College, London)

### Cleft palate repair

*M. Swan****, T. Goodacre**, Profesor J. Meakin*, Dr. D.G. Bucknall***, Dr. J.T. Czernuszka, N. Rounthwaite*

The project aims to create a tissue expander to repair cleft palates and other similarly anisotropic congenital deformities. The project will also examine the mechanical properties of mucosa and dermal tissues to gain an insight into their expansile properties. (*Nuffield Dept of Surgery, **Dept of Plastic Surgery, ***Georgia Tech, USA, ****Salisbury General Hospital)

### Crystallographic texture determination of calcium phosphates

*Dr. P. Fewster*, Dr. J.T. Czernuszka*

Novel off-axis X-ray diffraction techniques and modelling are being used to determine phase orientation, morphology and purity. Comparison with other techniques will be made throughout. (*Philips Research Labs)

### Musculoskeletal tissue regeneration

*Dr. J.T. Czernuszka, D. Wahl, R. Walton, Professor J.T. Triffitt*, Z. Dao*, Professor R. Oreffo**, J. Dawson **, Professor A. El Haj ***, Dr. S. Cartmell ***, G. Jones ****

Bone is a highly vasucalarised and is the most transplanted tissue after blood. These sets of projects aim to highlight the issues which need to be addressed to regenerate bone, cartilage tissue and hybrid structures.(*Nuffield Dept of Orthopaedic Surgery, **Southampton University. ***Keele University)

### Design and fabrication of ceramic: biochemical: polymer composites

*Dr. J.T. Czernuszka, Professor E. Bres*, Professor W. Hosseini***

Additions of bio-chemicals, such as amino acids or lipids, either to the growth medium or onto the surface of polymeric substrates influence strongly the morphology and crystallographic orientation of deposited ceramics. This is being used to create tailored composites and structures.(*University of Lille; **University of Strasbourg)

## III - POLYMERS

### Vacuum Web processing

*Dr. H.E. Assender, Dr. J. Topping, Dr. B.M. Henry*

We have recently purchased a unique vacuum web processing capability. The coater can run a 30cm polymer web at speeds of up to 5m/s to allow the deposition of multiple layers from the following sources: i) aluminium evaporator, ii) dual magnetron sputter, iii) plasma iv) flash evaporation of organic materials with UV cure. Films can be produced for applications such as controlled optical properties and surface finish, high and low energy surfaces, barrier layers or biocompatibilisation.

### Nanopatterning of block copolymers

*C. Copplestone, Dr. H.E. Assender, Professor R. Register**

Thin films of diblock copolymers make excellent contact masks for surface patterning, which have been employed to create dense arrays of metallic and semiconductor quantum dots or lines spaced only a few tens of nanometers apart. Future directions for this project will include elucidation of the mechanism and kinetics of the alignment process, and the factors controlling them. (*Princeton University, USA)

### Surface crystallisation of polymers

*K. Shinotsuka, Dr. H.E. Assender*

Under controlled annealing conditions, novel crystalline morphology has been observed in heat-treated PET films. This may be associated with a depressed surface glass transition temperature allowing surface-specific crystallisation processes. We are investigating this observed phenomenon further with a wider range of polyester materials to establish the origin of the observation. (Funded by Oji Paper Co Ltd.)

### Transparent vapour barrier systems on vacuum-planarized polyester films

*H. Suttle, Dr. B.M. Henry, Dr. H.E. Assender*

Use of the polymer web coater to deposit under vacuum gas barrier layers combining vacuum deposited organic and inorganic materials. Study of the influence of layer thicknesses, number of layers and composition on the characteristics of the layer. Determination of the barrier properties by existing (Wilton Ca test) or novel permeation methods along with examination of other properties of deposited layers such as adhesion, friction, colour etc.

### *Understanding Bioselective Surfaces and their Medically Relevant Ligands*

*Dr. D.G. Bucknall*, H. Womersley, D.J.T. Vaux***

This project is an interdisciplinary study of the surface interactions of medically important proteins and cell membranes with defined polymer surfaces. The project involves the application of molecular biological techniques to generate constrained peptide libraries for screening interactions with specially prepared defined polymer surfaces. Candidate peptide-surface interactions will be further characterised by both physical and cell biological methods. (*Georgia Tech, USA; **Dunn School of Pathology, University of Oxford)

### *Long range ordering of block copolymer*

*Professor R. Register*, Dr. P. Chaikin*, J. Waller, Dr. D.G. Bucknall**, Dr. P.J. Dobson*

Block copolymers are being actively studied due to their inherent self-assembly characteristics, from which well defined repeating or crystallographic structures can be produced. The ability to control these structures over large length scales necessary for making useful devices has yet to be developed and this project is part of a larger effort to achieve this goal. One of the principle objectives of the research is to investigate methods for producing long range lateral ordering of spherical phase forming block copolymers in thin polymer films. A number of methods will be investigated including use of applied electric or magnetic fields as well as thermal gradients, all of which are known to influence the structure of copolymers. The external fields will be applied to the copolymers whilst they are in the melt state and above the order-disorder phase transition, and should allow us to impose long range ordering behaviour desired. In order to understand how to control this field induced ordering a wide parameter space in terms of copolymer molecular weight, film thickness, annealing temperatures, field strength and surface topography of the substrate will be investigated. (*Princeton University, USA; **Georgia Tech, USA)

### *Polymer based barrier materials*

*P. Islam, Professor C.R.M. Grovenor, Dr. H.E. Assender, R. Hammond-Smith**

Thin film barriers to oxygen and water are critical components in a very wide range of industrial application, including display technologies, polymer electronics and packaging. This project will investigate the potential of a family of reactive liquid crystal coatings on polymer substrates, focussing on defining the relationships between the liquid crystal components, processing methodology, resulting phases and mesostructure, and permeation barrier properties. (*Merck Chemicals Ltd)

### *Polymer nanocomposite materials*

*V. Chan, L. Taylor, Dr. H.E. Assender, Dr. L. Figiel*, Professor F. Dunne*, Dr. C.P. Buckley*, Dr. J Sweeney**, Professor E. Harkin-Jones****

Investigation of the microstructure and interfacial properties of PP and PET/clay nanocomposite materials. This is to provide information that will be used by others in the development of computer simulations of the processing of these materials. In particular we are interested in: i) the distribution of orientation in the polymer and in the clay particles (and any correlation between these) following various film drawing and annealing treatments, and ii) any modification of the polymer close to a clay particle in terms of its glass transition temperature, its mechanical properties and its crystallisation.(*Department of Engineering Science; **University of Bradford; ***Queen's University Belfast)

### *Selective Encapsulation of Fullerenes in Diblock Copolymers*

*J. Waller, Dr. D.G. Bucknall*, Professor G.A.D. Briggs, Dr. K. Porfyrakis, Dr. H.W. Beckham**

Using the selective solubility of fullerenes in some polymers, we are using diblock copolymers to create ordered networks of fullerenes. Using advanced NMR techniques together with neutron and X-ray scattering we are studying the behaviour of the fullerenes on the copolymer phase behaviour. Although at minor volume fractions of fullerene addition the copolymer phase behaviour is unmodified, the wetting behaviour of thin films of the copolymer is affected. (*Georgia Tech, USA)

### *Microstructure of polymeric materials*

*Dr. D. Vesely*

The structures of amorphous and crystalline polymers are studied by light and electron microscopy. New techniques, which overcome and/or utilize the electron beam damage are developed. These techniques, which include microdiffraction, STEM dark field imaging, mass loss measurements, selective staining and chemical analysis are used to obtain more information on the molecular arrangement in amorphous and crystalline polymers. The aim of this work is to understand the effect of micro-structure on the mechanical properties of polymer systems and composites.

# IV - PHOTOVOLTAIC MATERIALS

## The optoelectronics of organic photovoltaic materials.

*A. Barkhouse, Dr. H.E. Assender, P.L. Burn**

This work focuses on the design and characterisation of a nanocomposite organic/inorganic photovoltaic material. The optoelectronic behaviour of the various materials under investigation is being characterised (Supported by the Rhodes Trust and Toppan Printing Company Ltd.) (*Dyson Perrins Laboratory, Oxford University)

## Device manufacture and characterisation of organic photovoltaic materials

*Dr. K.R. Kirov, Dr. H.E. Assender*

Organic-inorganic nanocomposite photovoltaic materials are being designed and characterised. This work seeks to develop and characterise the combination of materials components that go to make up a polymer composite photovoltaic device, with particular emphasis on the organic components and interfaces, and to improve the device manufacturing processes for lab-scale testing. (Supported by EPSRC and Toppan Printing Company Ltd.)

## Modelling photovoltaic devices

*C. Martin, Dr. V.M. Burlakov, Dr. H.E. Assender*

Simulate the key elements in the operation of polymer composite photovoltaic devices. In particular we are investigating the role of microstructure and electric field effects on the charge transport in the composite material. (Funded by EPSRC and the Toppan Printing Company)

## Nanocrystal / polymer composites for photovoltaics

*R. Beal, A. Stavrinadis, Dr. A.A.R. Watt, Dr. H.E. Assender, Dr. J.M. Smith*

Composites of organic materials and inorganic semiconductor nanocrystals are being explored for use in photovoltaic (PV) devices. Such materials combine the advantages of inexpensive fabrication with fine control of the optical absorption spectrum. The principal challenge is to synthesize materials in which the photogenerated electrons and holes are separated and transported efficiently to the device contacts. We are engaged two areas of study; (i) fabricating nanocrystals in organic hosts as a means to produce ready-made composites in which photogenerated holes are extracted from the nanocrystal into the polymer, and (ii) investigating the use of nano-heterostructures (quantum dot quantum well nanocrystals) as a means to ‘engineer’ the properties of the absorption sensitizers and increase internal quantum efficiency (IQE). ct

# V - CARBON NANOMATERIALS

## Filling multi-walled carbon nanotubes with metals

*Dr. N. Grobert*

Carbon nanotubes (CNTs) can be filled with various materials. Generally a two-step process is used whereby CNTs are grown, opened via oxidation and subsequently are filled. Here we have developed a technique for the in-situ filling of CNTs using the pyrolysis of metal-organic precursors. Depending on the precursors pure metal-filled or alloy-filled CNTs can be produced. (Supported by The Royal Society)

## Understanding carbon nanotube growth

*Dr. N. Grobert, Dr. L.Y. Chang, Professor A.I. Kirkland*

Carbon nanotubes (CNTs) can be produced using different techniques, including carbon arc-discharge, laser ablation, electrolysis and chemical vapour deposition. Most of these techniques require metal catalyst particles. State-of-the-art electron microscopy techniques are used to investigate these metal particles and their role in CNT growth. (Supported by The Royal Society)

## *Aerosol production of arrays of pure carbon and N- or B-doped carbon nanotubes*

*Dr. N. Grobert*

Pure and well-aligned carbon nanotubes can be prepared in gram quantities using homogenously dispersed aerosols generated from metalorganic precursor solutions using an ultrasonic spraying device. In addition, this process can also be adapted for the synthesis of bulk amounts of nitrogen and boron doped carbon nanotubes and composites of carbon nanotubes with alumina, silicon carbide and other ceramic materials. SEM and TEM investigations reveal that the products are generally arranged in carpet-like flakes containing high yields of well graphitized polyhedral particles or amorphous carbon, which are major drawbacks of standard production methods. With this method it is now possible to explore the chemical and physical properties of, for instance, CNx nanotubes and their composite materials without the influence of by-products or the need of additional purification processes. (Supported by The Royal Society, STREP BCN-Tube European Commission)

## *One-dimensional crystal growth inside single-wall carbon nanotubes*

*Professor A.I. Kirkland, Dr. J. Sloan*, Dr. J.L. Hutchison, Professor M.L.H. Green***

Crystals of various salts and metals grown within single-wall carbon nanotubes are effectively 1-D wires, with a range of interesting physical properties which arise from their unique configurations, We are exploring ways of growing these structures, which are characterised by HREM, EDX and EELS. Their physical properties are also under investigation. (*Advanced Technology Institute, University of Surrey; **Inorganic Chemistry Laboratory) (Funded by EPSRC, Leverhulme Trust and The Royal Society)

## *Carrier transport of Fe-filled multi-walled carbon nanotubes*

*Y. Nakajima*, T. Fukuda* , Dr. N. Grobert, Professor T. Maekawa*, Dr. T. Hanajiri**

The pyrolysis of ferrocene:C60 mixtures yields Fe-filled multi-walled carbon nanotubes (MWNTs). Transport measurements are being carried out on Fe-filled and test devices are fabricated by means of lithography techniques used in semiconductor device processes. (*Bio-Nano Electronics Research Centre, Toyo University, Kawagoe, Japan) (Funded by The Royal Society, 21st Century's Centre of Excellence Programme - Bioscience and Nanotechnology)

## *Carbon nanotube reinforced ceramics*

*T.T. Chu, Dr. N. Grobert, Professor M.L.H. Green*, Dr. R.I. Todd*

There have been several attempts recently to make ceramic nanocomposites in which the reinforcing phase consists of carbon nanotubes. None has resulted in a viable composite, either because the nanotubes have been destroyed by the high firing temperatures used, or because the nanotubes have not been properly dispersed in the ceramic matrix. We are trying to solve these problems using a variety of techniques and using both single- and multi-walled nanotubes.

## *Formation of Growth of Hybrid Carbon Nanomaterials*

*Dr. M. Rossi*, Professor M.L. Terranova**, Dr. A.S. Barnard*

Investigation of a new class of hybrid nanocarbon materials characterized by uniform coatings of nanodiamonds (with diameters in the range 20-100 nm), nucleated and grown directly on single-walled nanotubes (SWNTs), and bundles of SWNTs up to 15 um long. Ordered arrays of rigid hybrid nanocarbon structures are grown in a modified CVD reactor by means of reactions between carbon nanopowders and atomic H. The interface structure, nucleation and crystallization/growth mechanisms of the nanodiamond coatings are being investigated using thermodynamic modeling, as well as ab initio Density Functional theory (DFT) and Density Functional tight binding (DFTB) computer simulations. The distribution and configuration of impurities in these structures are also under investigation. (*Dipartimento di Energetica, University of Rome La Sapienza; **Dipartimento di Scienze e Technologie Chimiche and MINASlab, University of Rome Tor Vergata) (Funded by Italian MIUR through the FIRB National Program with support from The Glasstone Trust)

## *Fabrication and microscopic analysis of carbon nanotube-reinforced metal thin films*

*C. Schurr*, Dr. A. Matveev*, Dr. J. Nucci*, Dr. N. Grobert, Professor E. Arzt**

Carbon nanotubes (CNTs) have been used as reinforcing materials for various composite materials including a number polymers and some ceramic materials. In this project we are investigating the feasibility to fabricate CNT metal matrix composites to study their mechanical properties. State-of-the-art electron microscopy is carried out to gain a better understanding of the CNT metal matrix interaction, which is vital to assess the assessment of the mechanical behaviour. (*Max-Planck-Institute for Metals Research, Stuttgart, Germany)

### *Bionanotechnology and carbon nanotubes: protein-functionalisation and biosensing*

*Dr. S. Contera*, H. Hamnett*, N. Toledo*, K. Voichovsky *, Dr. M. de Planque*, Dr. N. Grobert, Professor J. F. Ryan**

Small molecules, such as O2, NO2, and NH3, as well as larger protein molecules and DNA can adsorb onto carbon nanotubes (CNTs). The presence of such molecules can change the electrical properties of CNTs. In this project we are investigating the sensing behaviour in nitrogen-doped CNTs (which have been predicted to be metallic) when they are functionalized with metalloproteins. We have shown that proteins including, cytochrome c, ferredoxin, ferritin and azurin can be adsorbed onto nitrogen-doped nanotubes and imaged using Atomic Force Microscopy (AFM). These functionalised CNTs are integrated into circuits and I-V curves are being measured. (*Bionanotechnology IRC, Physics Department, University of Oxford)

### *Manipulation of carbon nanotubes using a rotational magnetic field*

*Dr. H. Morimoto*, Y. Nagaoka*, Dr. N. Grobert * , Professor T. Maekawa**

The manipulation of nano- and micro-particles, biological molecules and cells is a key technology for the operation of nano- and micro-electromechanical systems (NEMS/MEMS) and micro-total analysis systems (microTAS). Various manipulation techniques of magnetic particles using magnetic fields have been studied and developed in recent years. Magnetic particles tend to form chain clusters in a dc magnetic field since the magnetic dipoles are aligned in the direction of the field. It is also known that chain clusters are rotated in rotational magnetic fields under certain conditions. We have developed a novel method for manipulating both magnetic and nonmagnetic particles using a rotational magnetic field. The present method is applied to the manipulation of CNTs. (*Bio-Nano Electronics Research Centre, Toyo University, Japan) (Funded by The Royal Society, 21st Century's Centre of Excellence Programme - Bioscience and Nanotechnology)

### *Location and Coordination of Impurities and Defects in Nanocrystalline Diamond*

*Dr. M. Sternberg*, Dr. A.S. Barnard*

Density Functional tight binding (DFTB) methods are being used to calculate the potetial energy surface (PES) and to identify energetically preferred substitutional sites for the inclusion of experimentally relevant impurities and defects in particulate nanodiamond and bucky-diamond (of approximtely 2 nm in diameter), and nanocrystalline diamond grain boundaries. This includes explicit comparison of core regions with different crystallographically unique surface facets, facet edges, and corners, as well as the fullerenic shells in bucky-diamond structures. In addition to this the affect of the surface, edge and corner impurities on the distribution of charge is also under investigation; as is the shape dependence of the distribution of charge in undoped diamond nanoparticles of different sizes. (*Center for Nanoscale Materials, Argonne National Laboratory) (Supported by The Glasstone Trust)

### *Spin-active and optically-active carbon nanomaterials spin arrays*

*Dr. J.H. Warner, Dr. K. Porfyrakis, Dr. A.A.R. Watt, Dr. A. Ardavan*, Professor G.A.D. Briggs*

Carbon nanomaterials offer discrete quantum states that are candidates for embodying quantum information. In this project will shall synthesise endohedral fullerene species, and potentially nanotubes, using arc discharge and other techniques. We shall isolate materials via HPLC and characterize them via a range of techniques. We shall insert fullerenes into carbon nanotubes to make one-dimensional spin chains. We shall develop physical chemistry for functionalized fullerenes and supramolecular carbon nanomaterials. We shall undertake chemical and structural characterization, using techniques such as UV-vis-NIR spectroscopy and photoluminescence and CW ESR, NMR and mass-spectroscopy, and electron microscopy. (*Department of Physics)

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# C. Electronic Materials and Devices

## I - SUPERCONDUCTING MATERIALS

During the last few years very exciting advances have led to the development of new oxide materials which superconduct at temperatures up to 160K. The Department of Materials has been working for the past 10 years on fabricating and characterizing bulk and thin film materials in collaboration with other University Departments and Industry. The aim of this work is to develop reliable processing techniques for materials fabrication, to understand the fundamental relationships between microstructure and properties and to investigate the potential of these materials for commercial exploitation.

### *Microstructural characterisation of MgB2 superconducting wires and tapes*

*S. Latif, Dr. S. Speller, Professor C.R.M. Grovenor*

Superconducting ceramic samples fabricated in wire form are being characterised by X-ray diffraction and electron microscopic techniques. Of particular interest is the determination of the phase distribution and alignment, grain boundary structure and chemistry, and impurity phase chemistry in materials prepared both within the University and by a number of collaborators, and the correlation of these features with critical current measurements. SEM, XRD texture analysis and orientation imaging microscopy techniques are being used to study the key microstructural features.

### *Synthesis and microstructure of MgB2 powders and wires*

*C. Dancer, Professor C.R.M. Grovenor, Dr. R.I. Todd, Dr. P. Kovac*, Dr. T. Prikhna***

MgB2 is a most promising new superconducting material for high current applications at temperatures below 30K. We are studying new methods for the chemical synthesis of high quality MgB2 powder with controlled particle size and impurity content. At the same time we are collaborating with the Kovac research group in Slovakia on the analysis of the microstructure of high current wires fabricated with commercial starting powder. XRD, SEM and EPMA analysis are all key aspects of the work, with high resolution SIMS analysis of oxygen and H contents. (*Institute of Electrical Engineering, Slovak Academy of Sciences, **Institute for Superhard Materials, Ukraine). (Funding provided by EPSRC DTA studentship for CD.)

### *Growth of thick epitaxial films of Tl-2212 for novel THz device structures*

*M. Korsah, Dr. S. Speller, Professor C.R.M. Grovenor, Dr. P. Warburton**

Superconducting films of the highly anisotropic Tl-2212 phase provide a simple way of fabricating novel device structures containing a large number of precisely positioned Josephson junctions. This project is to grow Tl-2212 thin films with microstructures specially optimised for these devices. Optimising epitaxial growth quality in films with thicknesses greater than 1 micron is the key technical challenge of the project, and requires a very detailed understanding of nucleation and growth processes in these films. (Funded by EPSRC and in collaboration with University College London*)

### *Superconducting Metamaterials for Near Field Microscopy Applications*

*Dr. S.C. Speller, Dr. C. Stevens*, Professor D. Edwards*, Professor C.R.M Grovenor*

Novel Magnetic Resonance Microscopes have been designed to offer dramatic improvements in 3D imaging for medical and biological applications. A sub-wavelength tapered waveguide structure enables the sensing of local magnetic fields. This "metaprobe" is ideally fabricated from superconducting materials to maximise the sensitivity of the instrument. This research project is concerned with the demonstration of practical methods to fabricate these extremely challenging superconducting/dielectric composites. (*Engineering Dept., Univ. of Oxford).(Funded by Royal Academy of Engineering / EPSRC)

# II - SEMICONDUCTOR MATERIALS

## Secondary electron mapping of doped regions in semiconductors

*Professor E. Grunbaum*, Dr. P.R. Wilshaw*

The secondary electron (SE) signal in an SEM is used to produce 2-dimensional maps of doped regions in silicon and III-V semiconductors. SE images of cross-sections of doped heterostructures and laser devices reveal the type and extent of doping. Quantitative information about the observed contrast has been obtained experimentally. A model has been proposed and is being developed to account for the effect and new measurements are being made using energy filtering of the secondary electrons. (*Dept of Physical Electronics, Faculty of Engineering, Tel-Aviv University, Israel.)

## An improved bone-implant interface

*A. Walpole, Professor J. Triffitt*, Professor V. Baranauskas**, Dr. P.R. Wilshaw*

A new coating for metal implant prostheses is being developed. This entails bonding a layer of porous alumina to the metal surface and filling the pores with a bioactive material such as bioactive glass. It is hoped that in this way the strength of the interface between the bone and implant will be improved whilst the mechanical properties of the implant are maintained. The response of human osteoblasts to porous alumina and other implant materials is being characterised. (*Nuffield Orthopaedic Centre, Oxford. **Faculdade de Engenharia ElŽtrica e de Computa ‹o, Universidade Estadual de Campinas, Brazil)

## Impurities and dislocations in Si wafers

*C. Alpass, Dr. S. Senkader, Dr. R. Falster*, Dr. P.R. Wilshaw*

The interaction between impurities such as O, N and H and defects such as dislocations and precipitates in silicon is being studied. In particular the diffusivity of O and N in the range 350-850C is being investigated together with the locking of dislocations by impurities and the mechanism by which precipitates weaken wafers. Also under investigation is the dependence of oxygen diffusion on the position of the Fermi level. One of the aims of the project is to understand impurity-defect interactions so that stronger silicon wafers may be manufactured. (*MEMC Electronic Materials Inc.) (Funded by EPSRC, MEMC Electronic Materials Inc.)

## Room temperature light emission from silicon

*D. Stowe, K. Fraser, Dr. S. Galloway*, Dr. R. Falster**, Dr. P.R. Wilshaw*

It is now known that efficient near-band-edge luminescence can be obtained from silicon provided the concentration of non-radiative recombination centres is made sufficiently small. In this project dislocations are being used as gettering centres for impurities and conditions are being optimised to produce efficient room temperature luminescence. Different annealing schedules are being developed to optimise the gettering process. (*Gatan, UK; **MEMC Electronic Materials Inc.) (With support from MEMC Electronic Materials Inc.)

## Optically induced degradation of Cz-silicon solar cells

*C. Alpass, Dr. S. Senkader, Dr. R. Falster*, Dr. P.R. Wilshaw*

The efficiency of Cz-silicon solar cells degrades significantly on exposure to sunlight. In this project the influence of light on oxygen diffusion in silicon at low temperatures is being investigated. The purpose is to determine whether electron hole pairs generated by the illumination are responsible for enhanced oxygen diffusion. In collaboration with MEMC Electronic Materials Inc.(*MEMC Electronic Materials Inc.)

## Modeling the Formation of Semiconductor Quantum-wires

*N. Pradhan*, Dr. X. Peng*, Dr. H. Xu**, Dr. A.S. Barnard*

This project uses thermodynamic modeling and first principles density functional theory (DFT) computer simulations to investigate the formation mechanisms of high-aspect cadmium selenide (CdSe) and cadmium sulphide (CdS) quantum wires. Formation via the oriented-attachment or axial-growth mechanisms are considered. (* Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, 72701, USA; ** Department of Geology and Geophysics, and Materials Science Program, University of Wisconsin, Madison, WI, 53706, USA) (Supported by the Glasstone Trust, the National Science Foundation and the Graduate School of the University of Wisconsin - Madison.)

## *Spectroscopy of Quantum Dot Quantum Wells*

*E. Tyrrell, Dr. J.M. Smith*

Semiconductor nanocrystals are becoming increasingly important in a wide range of applications in fields as diverse as medicine, renewable energy, and telecommunications. Perhaps their most useful feature is that they absorb and emit light at wavelengths that is tuneable with the size of the nanocrystal. In most nanocrystals choosing the size also determines other important optical properties, such as the luminescence lifetime and linewidth, which can act as limiting factors in many applications. In this project we study novel nanocrystals, called quantum dot quantum wells (QDQWs), in which the aforementioned optical parameters may be tuned independently, leading to greater flexibility and enhanced functionality of the materials. The project involves optical spectroscopy (photoluminescence and photoluminescence excitation) of ZnS / CdSe QDQWs grown by collaborators at the University of Manchester. We model our data by calculating the electronic energy levels in the materials using a specialised 8-band Hamiltonian in spherical symmetry. Funding for this project has been provided by the University's Research Development Fund.

## *Fluorescence stability in semiconductor nanocrystals*

*B. Sher, Dr. J.M. Smith*

Semiconductor nanocrystals grown by wet chemical methods have enormous potential for use in optoelectronics applications such as photodetectors, light emitting diodes, and lasers. The unique quantum mechanical properties of electrons and holes in single nanocrystals may even be exploited to build such devices as single photon sources for quantum cryptography, or ‘qubits’ for quantum computation. A problem exists, however, in that if the surface of the nanocrystals is not well passivated, electrons and/or holes can escape from the nanocrystal into surface trap states, and cause random spectral drift and blinking in the luminescence intensity. In this project we study the fundamental carrier dynamics that lead to the instabilities in the luminescence from nanocrystals, and address ways to tackle the problem of surface passivation, including embedding the nanocrystals in thin films and studying novel "quantum dot quantum well" nanocrystals. Our characterisation techniques focus on photoluminescence spectroscopy and time-resolved photoluminescence of single nanocrystals. The project involves collaboration with Professor Paul O'Brien at the University of Manchester, and Professor Yoon Bong Hahn at Chonbuk University in S. Korea.

## *Dislocation Control in Silicon using Nitrogen Implantation*

*C. Alpass, Dr. S. Senkader, Dr. R. Falster*, Dr. A. Jain**, Dr. P.R. Wilshaw*

With the advent of advanced device technologies often involving heterostructures and strained layers there is an increasing problem with the generation and movement of dislocations in the near surface regions of Si wafers. This project is investigating the possibility of using ion implanted nitrogen as a high concentration source of electrically inactive nitrogen which can subsequently diffuse to and hence "lock" near surface dislocations so preventing the damaging effects that would be caused by their movement. In collaboration with Texas Instruments and MEMC Electronic Materials Inc. (*MEMC Electronic Materials Inc. **Texas Instruments, USA)

## *Semi-insulating Silicon*

*D. Jordan, Dr. R. Falster*, Dr. P.R. Wilshaw*

Advanced silicon devices are working at ever higher frequencies so that an increasing number of applications which presently use III-V materials could, in principal, now use silicon. However, at these very high frequencies free carriers in the silicon substrate serve to absorb microwave energy reducing the efficiency of the circuits as a whole, so prohibiting their use. This project is to investigate a novel way to produce semi-insulating silicon substrates which would then allow the full speed of silicon devices to be utilised. In collaboration with MEMC Electronic Materials Inc. (*MEMC Electronic Materials Inc.)

# III - MAGNETIC MATERIALS

## MBE growth of epitaxial tunnel junction structures

*C. Wang, Dr. A. Kohn, Professor A.K. Petford-Long*, Dr. R.C.C. Ward***

The MBE system in the Clarendon Laboratory is being used to grow epitaxial MgO based tunnel junction structures. The microstructure, chemical composition and electronic structure are being analysed using HREM and analytical TEM. We focus on the characterisation of the interface and its influence on the device properties. (*Argonne National Laboratory, USA, **Clarendon Laboratory, Oxford) (Funded by EPSRC)

## Microstructural characterization of Heusler alloys for spin electronic devices

*Dr. A. Kohn, Professor A.K. Petford-Long*, Dr. Z.H. Barber**, Dr. L.J. Singh**, Dr. L.F. Cohen***, Dr. W.R. Branford****

Thin layers of the Heusler alloy Co2MnSi are sputter deposited on GaAs(100). The potential to achieve full spin polarization in this alloy along with an excellent lattice match to GaAs make this system a promising candidate for spin injection application into semiconductors. The composition, crystallographic structure, and interface are characterized by high-resolution and advanced analytical TEM. This data then enables to understand the magnetic and transport properties of the film.(* Argonne National Laboratory, USA, **Department of Materials Science and Metallurgy, University of Cambridge, ***Blackett Laboratory, Imperial College)

## High spatial resolution analysis of TMR structures

*D. Kirk, Professor A.K. Petford-Long*, Dr. M.T. Kief**, Dr. A.A. Morrone**, Dr. B. Karr***

The first aim of this project is to develop advanced TEM characterisation techniques that are specifically tailored to the analysis of TMR structures. The second aim is to provide structural, microchemical and micromagnetic analysis of TMR structures, at nm to sub-nm resolution, as a function of deposition conditions, anneal conditions and oxidation conditions. These data will then be correlated with the bulk magnetic and transport properties of the TMR structures. (*Argonne National Laboratory, USA, **Seagate Technology) (Funded by EPSRC and Seagate Technology)

## In-situ TEM studies of magnetic domain structure

*Professor A.K. Petford-Long*, R.C. Doole*

Facilities are being developed for Lorentz microscopy of magnetic materials using a 400kV TEM. Facilities developed so far allow the effects of temperature and applied fields on the magnetic domain structure to be studied in situ using heating, cooling and magnetising stages, with the additional capability of observing active magnetoresistive elements in situ. The range of facilities is being further extended. (*Argonne National Laboratory, USA)

## Composite magnetic nanoparticle systems

*A. Eggeman, D. Forrest, Professor A.K. Petford-Long*, Professor P.J. Dobson**, Dr. R. Potter****

Composite systems containing magnetic metal nanoparticles have many technological applications. The aim of this project is to fabricate these materials using sol-gel processes, and to characterise their structure, composition, magnetic and transport properties. (*Argonne National Laboratory, USA, **Academic Director of the Oxford University Begbroke Science Park, ***Johnson Matthey) (Funded by EPSRC and Johnson Matthey)

## Development of an MRAM device embedded on silicon

*Dr. V. Lazarov, Dr. A. Kohn*

The EMAC project which stands for 'Embedded Magnetic Components' is unique in that it will integrate MRAM directly at the heart of CMOS. The EMAC project hopes to bring innovations in the field of embedded MRAM fabrication, thus paving the way to 65nm node. Strategic objectives are to drastically reduce the complexity of MRAM processing and to ensure technology scaling-down. One of the other main purposes of this project is to develop a reliable stack of ferromagnetic materials on thin oxide directly onto silicon.(http://www.emacproject.com - a collaboration between CRMCN-CNRS (Fr), CEA (Fr), FRAUNHOFER-IMS (Ge), ARC (Au), University of Oxford (UK), Spintron (Fr), Semitool (UK), UJF (Fr), Toplink Innovation (Fr). t

# IV – QUANTUM INFORMATION PROCESSING

## Measurement based quantum entanglement of solid state spin qubits

*F. Grazioso, Dr. J.M. Smith, Dr. P. Kok, Dr. B. W. Lovett, Dr. S.C. Benjamin*

Recent advances in the theory of quantum information processing have shown that high fidelity quantum entanglement can be generated between remote systems simply by performing measurements on them in a certain way. From a materials perspective this is a huge advantage over traditional QIP schemes, which require controlled interaction between two or more systems - usually on nanometre length scales - to generate the necessary entanglement. Here we are developing the capability to perform a basic quantum measurement from which a measurement-based entanglement apparatus will be built. The 'qubit' that we are measuring is the spin state of a negatively charged Nitrogen Vacancy (NV-) defect in diamond; a system that has been demonstrated to have excellent coherence properties and on which some exquisite single qubit manipulation experiments have already been performed. Our measurement technique involves 'single shot' optical excitation, whereupon subsequent detection of an emitted photon reveals the spin state of the NV-. The 'remote entanglement' scheme imposes some exacting conditions on how this measurement must be achieved, but could enable us to build a useful quantum computer sooner than we had previously thought! The project involves collaborations with Professor Steven Prawer at the University of Melbourne and Professor Richard Warburton at Heriot-Watt University. Funding is provided by the EPSRC and MoD through the QIP IRC, and by Hewlett Packard Laboratories in Bristol.

## ESR Study of Carbon Nanostructures for Quantum Computing

*L. Clark, Dr. J.L.L. Morton, Dr. A. Ardavan*, Professor G.A.D. Briggs*

Molecules of N@C60 have an exceptionally sharp ESR signal corresponding to long-lived electronic spin states. The suitability of these states for storing quantum information is being evaluated. A chain of interacting spin-active molecules may be realised by filling a carbon nanotube. The possibility of using such a chain for processing quantum information is being considered. A pulsed ESR X-band spectrometer is being implemented. See www.nanotech.org (*Department of Physics) (Funded by EPSRC Foresight LINK Project, DTI and Hitachi Europe).

## Architectures for Computation in the Quantum Regime.

*Dr. S.C. Benjamin*

This project is concerned with the question, what is the best (most natural) architectural scheme for processing information at the quantum level? The issue is examined in two distinct contexts: processing classical information (bits) with quantum-scale structures, and processing of true quantum information (qubits). Although there are many topics of interest within this area, research into the ""global control"" concept is currently of primary interest. Using this approach bit/qubits can be effectively manipulated even if they are too close together to address individually. However, fundamental issues must be addressed before this novel paradigm can be considered mature: to determine the minimum space/time costs implied by adopting such a scheme, to quantitatively analyse fault tolerance (esp. for QIP), and to understand relative merits of one-, two- and three-dimensional arrays. (Funded by The Royal Society)

## Logic Gates with Excitons and Spins in Quantum Dots

*A. Kolli, E. Gauger, Dr. B.W. Lovett, Dr. S.C. Benjamin, Professor G.A.D. Briggs, Dr. J. M. Smith, Professor J. H. Jefferson*

We have shown that excitons in self-assembled quantum dots are suitable candidates for use in quantum information processors. Based on this, we have proposed two methods for the ultra-fast manipulation of coupled dot states: one exploits the optical Stark effect to entangle excitonic states of two adjacent quantum dots, the other uses a single delocalised exciton to generate an effective coupling between spins localized on each dot. Both schemes may be generalized to perform arbitrary single- and two-qubit quantum logic gates. We now aim to apply our formalism to optically and spin active carbon based nanostructures, as well as to quantum dots placed inside optical micro-cavities. We are also investigating methods for performing the quantum gates adiabatically, since this may improve decoherence properties. (In collaboration with Hewlett Packard Laboratories Bristol and Griffith University, Brisbane, Australia)

## High fidelity operations on electron spin qubits

*Dr. J.J.L. Morton, Dr. A. Tyryshkin**, Dr. A. Ardavan*, Professor S.A. Lyon**, Professor G.A.D. Briggs*

An increasing number of quantum computing implementations are turning to electron spin as the embodiment of a quantum bit (qubit). The ability to measure and reduce systematic errors in electron spin rotations is therefore crucial when evaluating such quantum computing proposals. We have developed pulsed electron paramagnetic resonance (EPR) sequences that can be used to measure precisely even small systematic errors in rotations of electron-spin qubits. Using these sequences we hope to demonstrate the ability to substantially reduce these errors using composite pulse sequences, allowing high-fidelity qubit operations to be performed.(*Clarendon Laboratory, Oxford University; **Electrical Engineering Department, Princeton University)

## Manufacture of HPLC Columns for Separation of N@C60

*J. Zhang, Dr. A.N. Khlobystov*, Dr. K. Porfyrakis, Dr. A. Ardavan**, Professor G.A.D. Briggs*

N@C60 and C60 are difficult to separate, as they have virtually indistinguishable affinities for most materials. We have targeted their most apparent difference, mainly that N@C60 is more polarizable than C60, to facilitate separation of the two molecules. We are designing materials that have exceptionally large polarizabilities and attaching them to silica for use as packing material for high performance liquid chromatography columns.(*University of Nottingham; **Clarendon Laboratory, Department of Physics)

## Optically detected magnetic resonance for single qubit readout

*Dr. G. Dantelle, Dr. A.A.R. Watt, Dr. J.J.L. Morton, Dr. K. Porfyrakis, Dr. A. Ardavan*, Professor G.A.D. Briggs*

In any electron-spin based quantum computer you need to be able to read out a single electron spin. We shall investigate techniques of optically detected magnetic resonance (ODMR) in the search for spin-dependent optical transitions in carbon nanomaterials. We shall undertake advanced optical spectroscopy and photoluminescence of endohedral fullerenes and other molecules, combined with ESR to perform ODMR spectroscopy, with a view to developing a technique for optical measurement of a single spin.(*Department of Physics)

## Towards Optical Readout of a Fullerene Quantum Computer

*A. Tiwari, Dr. A.A.R. Watt, Dr. J.J.L. Morton, Dr. K. Porfyrakis, Dr. A. Ardavan*, Professor G.A.D. Briggs*

We are developing materials and techniques to read out a spin qubit embodied in an endohedral fullerene spin state via optical means. We focus on magnetically and optically active fullerene species, and have demonstrated magnetic splitting of luminescence spectral lines from a candidate fullerene species, as well as direct optical interaction with an incarcerated ion. Combining these results with the results of pulsed electron paramagnetic resonance and pulsed optical spectroscopy, as well as theoretical studies of the quantum level structure, will develop a scheme to perform the readout. (*Department of Physics)

## Zeptolitre Reaction Vessels

*Dr. A.N. Khlobystov*, Dr. A. Ardavan**, Professor G.A.D. Briggs*

We are studying chemical reactions inside single walled carbon nanotubes (SWNTs). We have been able to efficiently fill SWNTs with a variety of reactive molecules. These molecules can react inside SWNTs to form a polymer of fullerene oxide with improved topology over the bulk polymer. The use of single-walled carbon nanotubes as reaction vessels is recognized by the Guinness Book of World Records as the smallest test-tube. (*University of Nottingham; **Clarendon Laboratory, Department of Physics)

## Decoherence of Confined Excitonic States

*Dr. B.W. Lovett, A. Kolli, E. Gauger, Dr. S.C. Benjamin, Professor G.A.D. Briggs*

We are investigating the primary decoherence mechanisms by which quantum information is lost to its surroundings from confined excitonic states. The confinement might be due to a synthetic nanostructure such as a quantum dot, or to a molecular unit, such as a fullerene. The decoherence is caused by interactions with phonons or by emission of photons. We are using a variety of methods to study these effects, varying from simple Markovian master equations (in which the environment is assumed to have no memory), to more complex non-Markovian approaches, which use the spin-boson model. We are also looking at ways in which we can increase the coherence time of molecular devices; for example, this might be done by using tailored laser pulses to perform quantum manipulations, or by designing environments which do not support particles which interact most strongly with our quantum bits. (In collaboration with Hewlett Packard Laboratories Bristol)

### Molecules inside Nanotubes: a Synergistic Host-Guest System

*Dr. A. Wolf, Dr. A.N. Khlobystov*, Dr. K. Porfyrakis, Professor G.A.D. Briggs, Dr. A. Ardavan*, Dr. J.G. Wiltshire*, Dr. L. Li*, Dr. R.J. Nicholas**

We are exploring interactions between carbon nanotubes and various organic and organometallic molecules, including fullerenes. These nanostructures demonstrate unique synergistic host-guest properties. Structural and dynamic behaviour of the encapsulated molecules is substantially affected by confinement in the nanotube and is mainly controlled by geometrical parameters of the host. Complementarily, the mechanical and electronic properties of the tubular host are influenced by the guest molecules due to the coupling between the molecular orbitals of the guest and the electronic bands of the nanotube. Host-guest systems of this type exhibit a range of functional properties which can be exploited in chemistry and nanotechnology. (*University of Nottingham; **Clarendon Laboratory, Department of Physics)

### Pulsed electron spin resonance to demonstrate entanglement and spin propagation

*Dr. L. Xiao, Dr. J.J.L. Morton, Dr. A. Ardavan*, Professor G.A.D. Briggs*

A key component of quantum information processing is the ability to propagate information along spin chains. Several theoretical schemes have been proposed for doing this. We shall use pulsed electron spin resonance of arrays of electron spins to investigate the effects of interactions and propagation of information along a spin chain.(*Department of Physics)

### Cluster-state quantum computing in quantum optics

*Dr. S.C. Benjamin, Dr. D. Browne, Dr. P. Kok, Dr. B. Lovett, E. Campbell, P. Danvirutai, J. Fitzsimons, A. Kolli, Professor G.A.D. Briggs*

Cluster-state quantum computing is a recent alternative to circuit-based quantum computing. It seems particularly suited for physical implementations that offer only probabilistic gates, such as linear optical quantum computing. Recently, the cluster-state formalism was adopted to show how quantum computing can be implemented in isolated quantum systems with optical transitions. This project encompasses the theoretical study of creating cluster states efficiently, and the effects of physical noise on its quantum computing capability.

### Endohedral Fullerenes for Quantum Information Processing

*Dr. J.J.L. Morton, Dr. K. Porfyrakis, Dr. A.M. Khlobystov*, Dr. A. Ardavan**, Professor G.A.D. Briggs*

One of the most remarkably robust examples of an unpaired electron spin within a molecule is that of a nitrogen atom trapped inside a spherical fullerene (termed N@C60). We have measured the coherence time of a qubit encoded within this electron spin system and performed single qubit operations using pulsed electron paramagnetic resonance (EPR). We are investigating the synthesis of several types of endohedral fullerene dimers including directly-bonded and oxygen-bridged dimers. These multi-qubit systems will then be characterised by EPR. We shall study the ability to control qubit interactions through the inter-fullerene bridge, and move on to investigate larger qubit arrays. (*University of Nottingham; **Clarendon Laboratory, Department of Physics)

### Dimers for quantum computing

*J. Zhang, Dr. K. Porfyrakis, Dr. A. Ardavan*, Professor G.A.D. Briggs*

Electron spin active dimers could be used to realize a two-qubit system for quantum computing. We have synthesized directly bonded empty fullerene dimers by high speed vibration milling. The same method can be used to synthesize endohedral fullerene dimers to realize a two-qubit system. We are investigating the switchable dimers for a controllable two-qubit system. We are synthesizing azobenzene bridged nitroxyl free radical dimers and fullerene dimers. UV/Vis light can be used to switch the bridge from trans- to cis-, or vice verse, in order to control the qubit interaction, which can be probed by ESR method. (*Clarendon Laboratory, Department of Physics)

### Graph States and Projective Measurement Based Quantum computation (theory)

*Dr. S.C. Benjamin, Dr. D. Browne, Dr. P. Kok, E. Campbell, P. Danvirutai, J. Fitzsimons*

Graph state (or Cluster-state) quantum computing is a recent alternative to circuit-based quantum computing. It seems particularly suited for physical implementations that offer only probabilistic gates, such as linear optical quantum computing. Recently, the cluster-state formalism was adopted to show how quantum computing can be implemented in isolated quantum systems with optical transitions. This project encompasses the theoretical study of creating cluster states efficiently, and the effects of physical noise on its quantum computing capability. (In collaboration with Imperial College, London) (Supported in part by the QIPIRC (see www.QIPIRC.org), and by the Royal Society.)

### *Controlled Entanglement of Fullerenes in Single Walled Nanotubes*

*S. Hu, Dr. A.A.R. Watt, Dr. A. Ardavan*, Professor G.A.D. Briggs*

Single walled carbon nanotubes can carry electrons very long distances without disrupting the direction of magnetic moment. This project will investigate the communication between mobile electrons in a nanotube with static electrons, localized nearby, that might act as repositories of quantum information. For example, the static electrons might reside on other chemical species introduced inside the nanotube in a filling experiment. (*Clarendon Laboratory, Department of Physics)

### *Multi-partite Entanglement in Quantum Information Processing*

*K. Loukopoulos, Dr. D.E. Browne, Dr. D. Jaksch**

This project will focus on understanding the properties of multi-partite entanglement in the context of quantum information processing and the efficient simulation of many-body quantum systems. In particular, new formalisms for the description and analysis of such states will be developed, beyond the well-established stabilizer and matrix-product-state formalisms. Applications of this theory to quantum information processing will be explored, not limited to quantum computation, but also including high-precision measurement and quantum clocks. A further application of this work will be the investigation of the multi-body entanglement present in naturally occurring many-body systems - with implications for the efficient desciption and (classical) simulation of such systems. This project is supported by the QIPIRC. (*Clarendon Laboratory, Department of Physics)

### *Electrically detected magnetic resonance and electron spin resonance in microwave stripline cavities, and development of methodology to control spin-spin interactions in arrays*

*Dr. R. George, Dr. J.J.L. Morton, Dr. A.A.R. Watt, Dr. A. Ardavan*, Professor G.A.D. Briggs*

Electrically detected magnetic resonance (EDMR) offers a means to study the interaction of stationary electron spins with conduction electrons. We shall use electrical measurements of arrays of spin-active species to evaluate the interaction of transport electrons with static spins in EDMR. We shall create microwave resonant cavities in striplines to perform ESR on small numbers of electron spins in 1-, 2-, and 3-D arrays. We shall investigate the feasibility of extending this approach to single electron spin measurements.(*Department of Physics)

### *Metals in carbon cages for quantum nanotechnology*

*S.R. Plant, Dr. K. Porfyrakis, Dr. A.A.R. Watt, Dr. J.J.L. Morton, Dr. A. Ardavan*, Professor G.A.D. Briggs*

Endohedral metallofullerenes incarcerate one or more metal atoms in a cage of (usually) 82 carbon atoms. Some of them are known to demonstrate high quality electron spin spectra, and we have recently been studying their photoluminescence spectra as a function of the excitation energy. The search is now on for metallofullerenes that exhibit coupled spin and optical properties as candidate materials for quantum nanotechnology. (*Department of Physics)

### *Molecular Architectures Templated by DNA*

*Dr. A. Ardavan*, Dr. S.C. Benjamin, Professor G.A.D. Briggs, Dr. R. Goodman*, Dr.A.N. Khlobystov**, Dr. J. Malo*, Dr. A. Turberfield**

We aim to establish a technology capable of using self-assembling DNA scaffolding to create functional architectures of molecular-scale components with the potential to perform computation. In our preferred system quantum information will be embodied in electron spins on atoms doped within fullerene cages, which are attached to a DNA lattice by covalent bonding. (*Clarendon Laboratory, Department of Physics; **University of Nottingham)

### *Supramolecular structures for nanoelectronics and quantum computing*

*A. Shaw, Dr. F. Silly, Dr. M.R. Castell, Professor G.A.D. Briggs, Dr. A. Ardavan*, Dr. S.C. Benjamin, Dr. K. Porfyrakis*

Conventional lithographic techniques for surface patterning have powered technological progress for decades and can now reach dimensions down to 20-30 nm. We shall pursue a fundamentally different approach to templating based on a 'bottom-up' nanotechnology in which nanoscale building blocks spontaneously adopt an ordered configuration through a self-assembly process. We shall use these templates to create structures suitable for nanoelectronics and quantum computing. The primary approach will be deposition of a passive molecular 'scaffolding' followed by subsequent deposition of a molecular species that forms an ordered distribution within that scaffolding. The species employed will be an endohedral fullerene with the property that the encapsulated atom can store information in the state of its nuclear and/or electron spin. In this way we shall create ordered arrays of quantum bits (qubits). Experiments will be designed to characterise the qubit-qubit intereactions, and the results will be used to guide further generations of nanoarray synthesis, with the ultimate goal of creating structures suitable for information processing. (*Department of Physics)

### *Theory and modelling of nanotubes and fullerenes for quantum information processing*

*L. Ge, Dr. B. Montanari*, Professor J.H. Jefferson**, Professor D.G. Pettifor, Professor G.A.D. Briggs*

For the implementation of a quantum information processing (QIP) device, ab initio Hartree-Fock and density functional calculations are performed to predict the electronic structure, charge distribution, geometries, and energetics in nanotube-fullerene systems. These include charged C60, alkali metal fullerides, Sc@C82, La@C82, Y@C82 and nano peapods (i.e. single-wall carbon nanotubes containing fullerenes or endohedral fullerenes). The project is in collaboration with the Cambridge Hitachi Laboratory and the Cavendish Laboratory where the relevant QIP devices will be produced. The results will be used to parameterise correlated electron models to describe spin-qubit interactions in peapod structures (cf. the project of M Habgood et al.). (*CCLRC Rutherford Appleton Laboratory; **QinetiQ) (Funded by Oxford University Clarendon Scholarship and St Anne's College Scholarship)

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# D. Processing

## Direct chill casting of Al alloys

*Dr. K.A.Q. O'Reilly*

A one tonne direct chill (DC) caster has been installed in the department and is being used to investigate the effects of alloy composition, processing parameters and grain refinement practice on the microstructures and properties of Al alloys.

## Sedimentation studies in Al alloys

*S. Srimanosaowapak, Dr. K.A.Q. O'Reilly, Professor J.D. Hunt*

Sedimentation studies are being developed to (i) investigate the effects of impurities, grain refiners and melt cleanliness on heterogeneous nucleation in commercially relevant Al alloys; and (ii) remove impurities and inclusions from melts in order to improve melt cleanliness. (Supported by the Royal Thai Government)

## The effect of grain refiner poisoning on intermetallic selection in 6xxx series Al alloys

*A.C.M. Lui, Dr. K.A.Q. O'Reilly, Dr. I.C. Stone*

In addition to their grain refining effect, commercial titanium diboride based grain refiners can also affect the selection of Al-Fe-Si intermetallic phases during solidification of Al alloys. Additions of Zr or certain other elements can poison the grain refining effect. Recent work has shown that the presence of Zr also affects intermetallic selection. This project will investigate the mechanisms determining intermetallic selection in these materials. (EPSRC)

## Nanostructured Al-based Alloys for high strength applications

*Dr. M. Galano, Professor F. Audebert*, Professor G.D.W. Smith*

Al-based nanostructured materials containing high volume fractions of quasicrystalline dispersoids are being produced by rapid solidification techniques. Particular emphasis is being placed on studying the microstructure stability and the mechanical properties leading to the manufacturing of the alloy in bulk shape. This project forms part of a collaboration agreement between the University of Oxford and University of Buenos Aires. (* University of Buenos Aires, Argentina)(Partially funded by Niobium Products Company CBMM)

## Development of new applications for freeze cast near net shapes

*N. Gregory, Professor P.S. Grant*

Freeze casting allows relatively dense ceramics to be made without the need for high temperature sintering. When casting is performed under vibration, the freeze-cast slurry behaves thixotropically and viscosity is reduced sufficiently to allow the slurry to replicate fine surface features and complex shaped moulds. Where sacrificial moulds are used, the possibility arises for the manufacture of high dimensional accuracy with relatively complex internal features. In order to expand the possible range of applications for alumina based freeze cast geometries, various approaches to manipulating the ceramic thermophysical properties are being investigated, for instance by the mixing of novel constitutes into the ceramic matrix. In each case, new approaches to processing and their effect on microstructure and properties are under investigation.

## Bulk nanocomposites Al based alloys

*Dr. M. Galano, Professor F. Audebert*, Professor G.D.W. Smith, Professor P.S. Grant*

Development and processing of Al based nanocomposites alloys for high strength applications in bulk shape by several processing techniques, focusing on the processing, the microstructure; and the resulting mechanical properties; definition of new compositions and processing conditions for optimised alloys; and scale-up to billet sizes suitable for forging and component trials. (*University of Buenos Aires, Argentina)

## Spray formed Al-Li-Mg-Zr(Sc) alloys alloys for airframe applications

*Dr. S. Hogg, L. Thomas, Dr. I.G. Palmer, Professor P.S. Grant*

A state-of-the-art 80kg Al spray forming plant has been installed and commissioned in a dedicated laboratory. Research focuses on production and evaluation of low density Al-Mg-Li-Zr(Sc) alloys by spray casting; characterisation of microstructure; investigation of secondary processing on the development of the microstructure and the resulting mechanical properties; definition of new compositions and processing conditions for optimised alloys; and scale-up to billet sizes suitable for forging and component trials. (Funded by EPSRC, Joint Infrastructure Fund and BAE Systems and in collaboration with Southampton University, Imperial College, BAE Systems and QinetiQ).

## Novel high energy density high reliability capacitors

*X. Zhao, Dr. C. Johnston, Dr. H.E. Assender, Professor P.J. Dobson*, Professor M. Johnson**, Professor P.S. Grant*

Current capacitor technology significantly limits the temperature capability and electrical performance of power electronics relative to the "More Electric Airframe" systems requirements, which are emerging rapidly as a key priority for both aeroengine and airframe manufacturers. Novel capacitor materials combining high dielectric ceramics and high performance polymers are being developed for aero-engine applications, particularly within the more electric aircraft concept. Investigations include characterisation of the fundamental material properties using advanced analytical instruments, clean room characterisation of the electrical properties, development of fabrication routes, and modelling of behaviour for lifetime prediction. (Funded by IeMRC and MoD/dstl) (*Academic Director of the Oxford University Begbroke Science Park, **University of Nottigham)

## Control of temperature during vacuum plasma spraying

*Professor P.S. Grant, E. Davies*, Dr. S. Duncan**

Vacuum plasma spraying (VPS) is the injection of metal or ceramic powder (10-50microns) into a hot gas plasma that melts and projects the molten droplets at high velocity onto a substrate to form a coating or composite. In order to maintain the uniformity and material properties of the coating, it is important to regulate the temperature of the surface during the spraying process. This project concerns the measurement of the temperature of the coatings surface using pyrometry and infrared thermal imaging and the use of data to adjust the VPS process in real-time to control the required temperature. (In collaboration with *Department of Engineering Science and funded by EPSRC).

## Piston development for high performance cars applications

*Dr. M. Galano, Professor F. Audebert*, Professor G.D.W. Smith*

Optimization of processing and composition of nanostructured Al based alloys for the development of automotive parts undergoing high strength at elevated temperature working environment. (*University of Buenos Aires, Argentina)

## Advanced materials for plasma facing components (PFCs) in fusion devices

*G. Thomas, Professor P.S. Grant*

This project concerns the use of thermal spraying and other manufacturing techniques to produce thick coatings with through thickness variations in compositions that are optimised for service in first wall applications in fusion reactors. Tasks include evaluation of possible materials combinations for plasma facing components from the perspective of all major constraints due to plasma surface interactions, physical properties for heat removal, radiation damage, etc. Evaluation PFC materials will be manufactured in-house using processing strategies for thermal and stress control, and optimised adhesion, minimum porosity and surface roughness, etc. Some material combinations are novel and offer particular challenges for processing technologies. (Funded by UKAEA)

## Spray forming of novel aluminium alloys

*C. Banjongprasert, Dr. S.C. Hogg, Dr. I.A. Palmer, Professor P.S. Grant*

The potential of the spray forming process to manufacture a range of novel Al-based alloys is under investigation. These include new Al-Cu-Li-Mg-Zr-X alloys for strong and tough aerospace alloys, Al-Mg-Si-Li alloys for ultra low density, high stiffness applications and metal-metal laminate structures obtained by spray forming and extrusion. In each case, precise compositions have been chosen to take best advantage of the unusual solidification conditions during spray casting to obtain large scale billets for microstructural and mechanical assessment that cannot be obtained by any other process. Microstructural response during downstream processing such as extrusion, and where appropriate, ageing heat treatments is being studied by analytical electron microscopy, phase extraction and X-ray diffraction, together with phase diagram modelling and calorimetry. (Funded by Royal Thai Scholarshi)

## Squeeze casting and semi-solid processing of Al alloys

*Dr. I.C. Stone, Dr. K.A.Q. O'Reilly*

An UBE 350 tonne squeeze casting and semi-solid processing machine has been installed in the department and will be used to investigate the effects of alloy composition, and processing parameters on the microstructures and properties of squeeze cast and semi-solid processed Al alloys.

## Toxic metal replacement in aerospace applications

*V. Marques, Dr. C. Johnston, Professor P.S. Grant.*

Current environmental legislation restricting the use of toxic metals in manufacturing and service will make the continued use of metals such as lead, cadmium and hexavalent chromium increasingly problematic for the aerospace industry and the basic understanding and development of aerospace-relevant replacement technologies must begin now. This project is supported by a consortium of aerospace companies and is part of a larger project involving close collaboration with Loughborough University. Pb containing materials are used extensively in Pb-based solders for electrical connections on printed circuit boards and printed wiring boards. Commercial Pb-free products are available for non-aerospace sectors but the limits to their use in the much harsher aerospace environment are unknown. The objectives of this project are: 1. To investigate the reliability of Pb-free solders under electrical/thermal regimes relevant to the harsh aerospace environment; and 2. To develop basic understanding and numerical analyses describing the electrical reliability of toxic metal replacement materials. Task one will involve highly accelerated life testing on a dedicated rig followed by detailed microstructural assessment, especially morphological and phase changes at temperatures >100oC under electric field. These investigations will make use of the wide range of state-of-the-art microstructure and microchemistry analysis equipment available at Oxford including analytical electron microscopy and elevated temperature microindentation. Task two will involve finite element simulations of the transient heat flow and strain distributions in solder joints during thermal cycling, based on novel experiments to measure Pb-free materials constitutive behaviour under aerospace conditions. (Funded by EPSRC and an aerospace consortium)

## Rheocasting of Al alloys

*S.B. Park, Dr. I.C. Stone, Professor B. Cantor**

The recently developed slurry-on-demand UBE New Rheocasting process is being investigated. Slurries are being produced on a commercial UBE Rheocaster, and their microstructures are being characterized quantitatively in order to investigate the role of the individual process parameters on the morphology and scale of the primary Al phase. The mechanical properties of the slurries are being measured using thermal mechanical analysis (TMA) in order to correlate slurry microstructure with properties and castability. The results are being used to determine constitutive laws for semi-solid alloys. (*University of York)

## NanoComp

*Mr R. Turner, Dr. C. Johnston, Professor P.S. GrantMr R. Turner, Dr. C. Johnston, Professor P.S. Grant*

Nanoparticles can be used as the basis to manufacture new composite materials in which some of the special properties of the small particles can be combined with the ease of manufacture of a surrounding matrix to form materials with an designed balance of attractive properties. There are many existing examples of this approach such as the nano-carbon black that goes into car tyres. The key to realising the enormous potential for new products based on nanocomposites is to find a way of incorporating the nanoparticles into the surrounding polymers, glasses or metals to form the composite – in a way that is controllable, measurable, assurable, in commercial quantities and focused on real world applications. NANOCOMP has been formulated in response to the SEEDA Call for Proposals “Realising the Economic Potential of Emerging Nano - Material Technologies in the South East Region”. The project brings together: Oxonica, an innovative nano-powder producing SME with world leading expertise within the SE Region; the characterisation, processing and development facilities at Oxford University’s Begbroke Science Park; and VT Halmatic with focused commercial requirements to pull through technology for a new range competitive products. A range of other companies from the South East will also be involved as materials and service providers, and may join the core consortium as the project matures. The core thesis of this work is that the exciting balance of properties of nanoparticulate materials can only be realised commercially if nanoparticles can be integrated reliably and cost effectively into real devices and systems. The product focus of NANOCOMP is environmentally friendly nanocomposites incorporating specially designed nanoparticles to radically improve fire retardation and UV protection properties, for use in marine, construction and other high value added sectors. Core technological hurdles to be overcome are: • To design nanoparticulate materials with very well controlled properties; • To incorporate these nano-materials into matrices to produce nanocomposite materials with novel or enhanced properties; and • To demonstrate the performance of these new composite materials in practical application environments. (Funded by SEEDA)

## Melt conditioning of Al alloys

*Dr. K.A.Q. O'Reilly, Dr. I.C. Stone*

Developing novel thermal and chemical melt conditioning procedures for the control of microstructures during casting, providing evaluation and measurement technologies for the same.

# E. Surfaces and Interfaces

## Pitting of Stainless Steels

*J.M. Sykes*

The effects of composition and microstructure on initiation of pitting corrosion are being investigated by electrochemical methods.

## Corrosion performance of lightweight airframe alloys

*K. Holmes, Professor P.S. Grant, Dr. J.M. Sykes*

Al-Li based alloys have been manufactured by spray forming at Oxford with compositions designed to avoid the requirement for homogenisation, quenching and ageing to achieve intermediate/high strengths. Since these alloys do not rely on the various intermetallic precipitate phases associated with high strength 2XXX and 7XXX airframe alloys, they are expected to show improved environmental and corrosion resistance under some conditions. Spray formed alloy environmental performance is being studied and compared with standard airframe alloys, and issues regarding compatability, for instance with C reinforced composites.

## Atomic scale studies of solute transport along grain boundaries

*Dr. G. Sha, Professor A. Cerezo, Professor G.D.W. Smith*

In situ experiments will be performed to study diffusion of oxygen along interfaces in steels. The objective of this work is to understand how solute diffusion affects environmentally-induced degradation. (Funded by Ministry of Defence, in collaboration with Manchester University, Birmingham University and Johnson Matthey.)

## Growth of ultra-thin oxide films

*C. Wu, Dr. M.R. Castell*

Crystalline oxides such as SrTiO3 have vast potential as a material to be integrated in the next generation of microelectronic devices. This project is concerned with growth of these films with atomic level precision using Sr and Ti as elemental sources and single crystal Pd and Si as substrates. The films are being characterised with scanning tunnelling microscopy, electron diffraction, and electron and optical spectroscopies.

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# F. Characterisation

## I - SCANNING TUNNELLING AND ATOMIC FORCE MICROSCOPY

### Atomic structure of oxide surfaces

*Dr. M.R. Castell, Dr. A.T. Paxton*, Dr. C.F. McConville***

Through the combined use of scanning tunnelling microscopy, atomistic simulations, and ion scattering spectroscopy, the atomic surface structure of reconstructed perovskite surfaces is being studied. (*Queens University Belfast, **University of Warwick) (Funded by The Royal Society)

### Modelling secondary electron emission from surfaces with inequivalent terminations

*Dr. M.R. Castell, Professor A.P. Sutton**

Objects with more that one type of surface termination, where there is a difference in the workfunction or potential of the terminations, give rise to ""patch fields"". The influence of these fields on secondary electron emission will be modelled. (*Imperial College)

### The surface structure of SrTiO3 (001) reconstructions

*D.T. Newell, Dr. F. Silly, Dr. M.R. Castell*

Ever increasing miniaturisation of integrated circuit technology continues to be a critical capability for the microelectronics industry in order to increase functionality and fuel market expansion. One of the major challenges identified by the International Technology Roadmap for Semiconductors (ITRS) is the introduction of new materials into the manufacturing process. Within a 5 year timeframe there is a good prospect of replacing the materials of the current SiO2 transistor gate insulator in complementary metal oxide semiconductor (CMOS) devices. One of the major contenders for the material replacement is SrTiO3. The purpose of the project is to investigate the surface reconstructions of SrTiO3 and determine their influence on the growth of silicon on these surfaces. Atomic resolution imaging through scanning tunnelling microscopy (STM) is the main research tool. This work is sponsored by EPSRC and Oxford Applied Research.

### Nanostructures on the SrTiO3 (001) Surface

*D.S. Deak, Dr. F. Silly, Dr. M.R. Castell*

Atomically resolved scanning tunnelling microscopy of the SrTiO3 (001) surface reveals that certain treatments give rise to two types of self assembled nanostructures. The one dimensional structure type consists of perfectly straight lines that run in <100> directions and have a minimum separation of 2.4 nm. The other structures are dots that on closest packing form 2.4 nm x 1.6 nm arrays. It is proposed that both structure types are formed through nano-crystalline growth of non perovskite phases on the surface. Further structural characterization and spectroscopy on these surfaces is currently being carried out. (Funded by The Royal Society and EPSRC)

### STM of polar SrTiO3 reconstructions

B. Russell, Dr. F. Silly, Dr. M.R. Castell

There are certain surfaces of crystalline materials that cannot have bulk-like terminations because this would lead to an infinite surface dipole. These surfaces are called polar surfaces and the atoms on a polar surface undergo substantial surface reconstructions in order to eliminate the dipole. The aim of this project is to study at atomic resolution the reconstructions of the SrTiO3 (111) and SrTiO3 (110) and related surfaces. Scanning tunnelling microscopy and electron diffraction will be used to determine the surface structure and Auger electron spectroscopy and secondary ion mass spectroscopy will reveal the chemical composition. (Sponsored by EPSRC.)

### Growth and spectroscopy of metallic nanoislands

*Dr. F. Silly, Dr. D. Imeson*, Dr. M.R. Castell*

Nanometre sized metal islands on oxide supports are used in diverse applications from catalytic materials to gas sensors. Interaction between the oxide support and the islands, the island shape, the temperature dependence of island ripening, and molecular interactions with the islands are all active areas of study. The atomic structures of the islands are imaged with scanning tunnelling microscopy, and a variety of spectroscopic techniques are used to measure their electronic structure. (*DSTL)

### *Structure and electronic properties of titanate materials using TEM and STM*

*H. Marsh, Dr. M.R. Castell, Professor A.I. Kirkland*

Complex metal titanates exhibit a variety of unusual structural, surface and electronic properties. This project aims to carry out high resolution studies on a variety of doped titanate systems such as Nb doped SrTiO3 where we expect phase separation to occur at high dopant concentrations. By combining state of the art scanning probe and transmission electron microscopic techniques it will be possible to correlate electronic and structural properties of these materials with atomic scale resolution.

### *Atomic-scale studies on the growth of metals on GaN(0001)*

*Dr. C. Norenberg, Dr. M.R. Castell*

In the past ten years, gallium nitride technology and its device applications have been developed rapidly. The performance of these devices (e.g. LEDs, laser diodes and high-power transistors) relies on good metal-GaN contacts. This project is focused on atomic-scale studies on the growth of metals (Pt, Pd, Au, Ti) on the GaN(0001) surface using variable temperature scanning tunnelling microscopy in combination with spectroscopic techniques. Fundamental issues such as adsorption mechanism, wetting behaviour, growth modes and the influence of surface treatments are investigated.

### *Optical resonances of oxide nanostructures*

*M. Marshall, D.S. Deak, Dr. M.R. Castell*

Crystalline oxides such as SrTiO3 have vast potential as a material to be integrated in the next generation of microelectronic devices. It has recently been discovered in Oxford that certain surface treatments of SrTiO3 produce atomic scale nanostructures by subtly changing the ratio of Ti to Sr in the surface region. This project investigates the quantum confinement of electrons in these nanostructures, similar to the particle in a box problem in elementary quantum mechanics. Atomic resolution scanning tunnelling microscopy will be used to determine the size and distribution of the nanostructures, and spectroscopy techniques will show the degree of quantum confinement.

## II - FIELD-ION MICROSCOPY AND ATOM PROBE MICROANALYSIS

### *Scanning atom probe*

*N. Grennan-Heaven, T.J. Godfrey, Professor A. Cerezo, Professor G.D.W. Smith*

The requirement of a sharp needle specimen can limit the type of materials that can be analysed in the atom probe, and is especially problematic in the area of thin films. We are testing a new type of atom probe system, first proposed by Nishikawa (Kanazawa, Japan) in 1993, which uses a micron-sized extraction electrode to allow analysis of microtips formed in thin film materials. This new instrument will allow atomic-scale microanalysis of electronic materials and layered metallic films. (Funded by EPSRC and the Oxford nanoScience division of Imago Scientific Instruments)

### *Atom probe analysis of information storage materials*

*S. Pinitsoontorn, Dr. C.-Y. You, Professor A. Cerezo, Professor A.K. Petford-Long**

Thin metallic layered films with applications in information storage are being grown by sputter deposition and atom probe tips are being fabricated from these layers by FIB milling. The layer composition and interface nature are being studied using both three-dimensional atom probe analysis, in parallel with HREM studies of the crystal structure of the films. Experimental analysis of interface changes with thermal annealing is being compared with simulations of the interdiffusion process. (*Argonne National Laboratory, USA.) (Funded by EPSRC, DTI and the Oxford nanoScience division of Imago Scientific Instruments, in collaboration with Hitachi Global Storage Technologies.)

## Dynamical Ising model simulations of phase separation

*A. Morley, Professor A. Cerezo, Dr. G. Sha, Dr. J.M. Hyde*, Professor G.D.W. Smith*

Monte Carlo simulations based on the dynamical Ising model are being used to study the early stages of phase separation in simple alloys. The model is able to simulate spinodal decomposition in Fe-Cr, nucleation and growth in Cu-Co and Fe-Cu, and simultaneous ordering and clustering in Ti-Al. The results of the simulations are compared with experimental measurements of atomic-scale composition variations, as determined by the 3-dimensional atom probe (PoSAP). (*Nexia Solutions) (Funded by Rolls Royce)

## Early stages of precipitation in 6XXX automotive sheet

*M. Zandbergen, Professor A. Cerezo, Professor G.D.W. Smith*

The thermal response of 6XXX series aluminium sheet materials, as used in the automotive industry, is very sensitive to time at room temperature prior to ageing during the paint-bake process. The compositional variations during the early stages of clustering and precipitation are being studied on the atomic scale using three dimensional atom probe microanalysis. (Funded by the Netherlands Institute for Metals Research.)

## Catalytic atom probe

*Professor G.D.W. Smith, Professor A. Cerezo, T.J. Godfrey, Dr. T. Visart*, Professor N. Kruse**

A specially adapted atom probe, incorporating a gas reaction cell, has been developed in order to permit the atomic scale study of catalytic reaction processes. (*Free University of Brussels.) (In collaboration with Johnson Matthey) (Funded by the EPSRC)

## Thermal ageing of steels

*Dr. G. Sha, A. Morley, Professor A. Cerezo, Professor G.D.W. Smith*

The atomic-scale changes which take place in the microstructure and composition of pressure vessel steels during long term thermal ageing are being investigated by three-dimensional atom probe techniques. (Funded by Rolls Royce and EPSRC.)

## Studies of advanced electronic materials with a pulsed laser 3-dimensional atom probe

*M. Mueller, Professor A. Cerezo, Professor G.D.W. Smith*

Whilst the 3-dimensional atom probe technique is widely used for studying metallic alloys, the use of a high voltage pulse to remove atoms from the specimen surface limits the application of the technique in the area of semiconductors and highly resistive materials. However, laser pulsing can be used to overcome this problem. This project will investigate the use of laser pulsing in the 3D atom probe and its effect on the range of materials that can be analysed and the quantitativity of the results obtained. The instrument will be used to study specific problems in advanced electronic materials and devices, with materials being provided by a number of industrial collaborators. (Funded by EPSRC and the Oxford nanoScience division of Imago Scientific Instruments.)

## Atomic mechanisms of tempering in steel

*C. Zhu, Professor G.D.W. Smith, Professor A. Cerezo*

3D atom probe techniques are being used to follow the movement of carbon atoms and alloy elements during the tempering of steels.

# III - ELECTRON DIFFRACTION AND TRANSMISSION MICROSCOPY, SCANNING ELECTRON MICROSCOPY, X-RAY MICROSCOPY AND MICROANALYSIS

The Department has a comprehensive range of electron optical instruments for structural and chemical characterization on the atomic level. In addition to a number of routine transmission and scanning electron microscopes, there are several state-of-the-art instruments for:

## *High resolution electron microscopy (HREM)*

The Department's 400 kilovolt JEOL 4000EX (II) electron microscope, commissioned in 1989, has a point-to-point resolution of 0.16nm with an information limit approaching 0.12nm; this is currently better than any other conventional instrument in the UK. The technique of structure imaging is being used to elucidate disorder on the atomic scale in a wide range of variety of crystalline materials. This instrument is equipped with an on-line TV system and also full digital imager acquisition and processing..

## *Field-emission-gun high resolution electron microscopy (FEG-TEM)*

In 1999 the Department installed and commissioned the UK's first 300 kilovolt field-emission-gun high resolution electron microscope. This instrument, a JEOL 3000F, is fully equipped with a comprehensive range of advanced analytical facilities, including light-element sensitivity EDX, parallel electron energy loss spectroscopy (PEELS), energy-filtered imaging (GIF), an electrostatic biprism for electron holography, a high performance CCD camera and a piezoelectric, drift correcting specimen stage. With a capability of microanalysis and electron diffraction from areas down to <0.4nm in diameter, and a spatial resolution of 0.16nm, this instrument is being used in a wide range of applications, involving new nanostructured materials. Recent upgrade includes STEM and High-angle Annular Dark Field imaging.

## *In-situ high resolution analytical electron microscopy*

A 400 kV high resolution electron microscope (JEOL 4000EX) has been extensively modified so that it can be equipped with a low-field objective pole-piece for studies of magnetic materials. The instrument also has an on-line TV imaging and digital image recording system. With the low-field objective pole-piece, magnetic specimens can be studied under a controlled applied field or at elevated temperatures. Recent additions to the instrumentation enable magnetisation configurations to be mapped quantitatively**.**

## *Analytical electron microscopy (AEM)*

A Philips CM20, a 200 kV AEM with full analytical facilities, was installed in 1990. A unique feature of this instrument is an energy-dispersive X-ray system (EDX) with simultaneously usable twin detectors. One detector is a standard thin Be window type, capable of quantitative analysis of elements down to Na (Z=11). The other is a windowless detector capable of analysing for light elements down to B (Z=5).

JEOL 2000FX and 2010 microscopes are also available, providing an excellent range of analytical capabilities, including (on the 2010) an Oxford Instruments windowless X-ray detector optimised for light-element analysis.

## *Aberration-corrected high resolution electron microscopy*

As part of the Departmental JIF grant, the Department has commissioned the world's first electron microscope to incorporate two aberration correctors, in both the image-forming and probe-forming lenses. This microscope is installed in a specially built suite of rooms at the Begbroke site. Based on a JEOL 2200FS it extends our high resolution imaging capability to below the 0.1 nm level, and also enables us to carry out nano-scale analysis at the same level. The unique instrument also has an in-column electron energy filter (omega-type), an X-ray detector, and is fully equipped with high performance digital image recording.

### *Scanning electron microscopy (SEM)*

The JEOL JSM-840F field emission scanning electron microscope (FEG-SEM) was installed for the purpose of obtaining images of crystal defects in bulk materials using the electron channelling contrast imaging (ECCI) technique developed in the department. This machine can produce both images of single dislocations and electron channelling patterns (ECP) and is being used to investigate sub-surface dislocation arrays and networks in partially relaxed epilayer materials and also to study defect distributions around crack tips. A JEOL JSM-6300 scanning electron microscope has also been installed for electron diffraction experiments. This has a $LaB_6$ gun which gives a higher beam current but also a larger probe size. An electron back scatter diffraction (EBSD) system allows automated mapping of local crystal orientation.

### *Remote scanning electron microscopy (WebSEM)*

A JEOL 5510LV was installed at Begbroke in 2003, and is extensively used for the development of remote microscopy in collaboration with the Oxford University e-Science centre. It has a $LaB_6$ electron gun and operates between 0.5 and 30 kV. Using secondary electron imaging, the best resolution attainable on high contrast samples (Au on C) is 3.5 nm at 30 kV in high vacuum mode and 4.5nm in low vacuum mode.

Facilities available on this instrument include Conventional secondary electron imaging of surface topography in high vacuum mode; back scattered electron imaging with annular detector, for compositional contrast and channelling contrast imaging in high vacuum mode; direct digital image capture to PC; remote internet control; low vacuum mode with back scattered electron imaging allowing observation of samples in a variety of gas environments at pressures from 1 - 270 Pa.

### *High resolution scanning electron microscopy*

The new field-emission gun, scanning electron microscope (JEOL 6500F) is installed at Begbroke and has been configured to perform a wide range of materials characterisation. High resolution imaging can be obtained using an EHT range of 1-25 keV (5nm-1nm) and it is particularly useful for imaging uncoated, non-conducting samples such as polymers and ceramics. It is interfaced to energy dispersive x-ray analysis, cathodoluminescent spectroscopy and electron back-scattered diffraction ancillary equipment for specialised investigations.

### *Electron probe microanalysis (EPMA)*

The department made a successful joint proposal with Department of Earth Sciences to the 1997 Joint Research Equipment Initiative for a high-specification microprobe. The instrument chosen was a JXA 8800RL electron probe microanalyser with four wavelength-dispersive X-ray spectrometers, for high-volume, automated microchemical measurements. This instrument is particularly suitable for light element analysis and X-ray mapping. It was installed in October 1999. The microprobe will contribute essential microchemical information to a series of research projects investigating metallic, ceramic, composite, superconducting, biomedical and sedimentary materials. The overall objective of the research is to apply state-of-the-art microprobe techniques in an integrated way to synthetic and natural materials. The scientific and technological impact will range from the development of improved efficiency aeroengine components and new prosthetic bone implants to phases synthesised at ultra-high (earth's core) pressures and marine sediments related to global change and the environment.

### *Focused Ion Beam system (FIB)*

The department has recently installed an FEI FIB2000 TEM system that is being used for micromachining with a spatial resolution down to 12 nm, and for sample preparation of TEM and atom-probe samples from specific sites. The system includes gas injectors for enhanced etching of metals and insulators, plus deposition of Pt.

### *Secondary Ion Mass Spectrometry (NanoSIMS))*

A Cameca NanoSIMS50 has recently been installed as part of the Departmental JIF grant. This instrument is a state-of-the-art Secondary Ion Mass Spectrometry facility with exceptional lateral spatial resolution (100 nm) and with the excellent chemical sensitivity characteristic of the dynamic SIMS technique. The NanoSIMS is being applied to a wide range of problems in materials science (grain boundary and interface analysis, trace light element analysis in Ni and Al alloys (including a unique ability to perform precise H mapping), diffusion mechanisms in polymer blends and 3-D dopant mapping in semiconductor materials and devices. In addition, we are developing new collaborations in the chemical analysis of biological materials with colleagues in Oxford and elsewhere - the first of these being on the study of metal species in hyperaccumulator plants, and in the mapping of radiopharmaceuticals in human tissue samples.

### *Interfacial Materials : Computations and Experimental Multi-Scale Studies*

*Professor D.J.H. Cockayne, Professor A.P. Sutton+, Dr. C.M. Bishop, Professor M. Ruhle*, Professor M. Hoffmann**, Dr. M. Gautier-Soyer***, Professor R Podgorni ^, Professor M Finnis+, Professor P Gumbsch**, S-J Shih, Dr C.J.D. Hetherington, K Dudeck*

Interfaces between amorphous/glassy layers and crystalline materials are playing an increasingly important role in the properties of manufactured ceramics and composites, especially as they move towards the nanometre scale. The goal of this project is to achieve a complete computational and experimental description of the structure and basic properties of crystal/glass interfaces, for the purpose of improving materials properties. This project is a joint project funded by the EU between participants at *Max Plank Institute, Stuttgart, **University of Karlsruhe, ***CEA, Saclay, and Imperial College

### *Structure of amorphous materials*

*Professor D.J.H. Cockayne, Y. Chen, Dr. C. Lang*

Techniques for investigating the structure of amorphous thin films and small volumes of amorphous materials have been developed and are being widely applied to obtain the radial distribution function. These techniques are accurate for single element materials, but require further development in the case of alloys. In this project, methods for determining partial radial distribution functions using electrons are being investigated, using energy selected electron diffraction combined with atomistic modelling. Refinement procedures are being developed which will allow differentiation between alternative structural models.

### *Development of FIB machining technologies*

*Dr. Y. Huang, Professor D.J.H. Cockayne*

Development and application of focussed ion beam machining technology for the preparation of nano structures.

### *Quantum wires and dots*

*Dr. J.L. Hutchison, Professor P.J. Dobson*, Dr. G. Wakefield***

We are assessing methods of making semiconducting dots and wires with dimensions less than 10 nm. This project is a coordinated optical, electronic and structural assessment of these new materials. (*Academic Director of the Oxford University Begbroke Science Park,; **Oxonica Ltd.)

### *Disorder in complex oxides*

*Dr. J.L. Hutchison, Professor A.I. Kirkland, Dr. J. Sloan**

Disorder in a variety of complex oxide structures which include layered bismuthates, non-stoichiometric rutiles and tungsten oxides is being investigated by high resolution techniques using the Oxford JEOL 4000EX and 3000F ultra-high resolution instruments. (*Advanced Technology Institute, University of Surrey)

### *Polyhedral and cylindrical metal chalcogenides*

*Dr. J.L. Hutchison, Dr. J. Sloan*, Professor R. Tenne***

Closed polyhedral structures of the layered materials WS2, MoS2 and other chalcogenides have recently been discovered. They are in the form of concentric, polyhedral shells, somewhat similar to the 'buckyball' and 'fullerene' carbon cage compounds. Their formation and structures are being investigated by high resolution electron microscopy. Their possible use as high-performance solid lubricants is being investigated. (*Advanced Technology Institute, University of Surrey; **Weizmann Institute, Israel)

### *Investigation of carbon nanotubes produced by novel synthetic methods*

*Dr. J.L. Hutchison, Dr. J. Sloan*, Professor N.A. Kiselev***

We are investigating the structure of carbon nanotubes prepared by various synthetic routes with the aims of controlling tube dimensions, and understanding growth mechanisms. (*Advanced Technology Institute, University of Surrey; **Institute of Crystallography, Russian Academy of Sciences)

### *Multivariate analysis of EDS and EELS data*

*Professor J.M. Titchmarsh*

The generation of large data sets by EDX and EELS imaging and spectroscopy is now routine using modern analytical TEM methods. However, conventional processing of data cannot separate small signals from artefacts and noise and cannot always detect correlations between signals. Multivariate analysis methods are being developed for routine handling of large data sets to improve the extraction of information from analytical EM data. (In collaboration with AEAT and INSS)

## Tilt- and through-focus series image reconstruction techniques for super-reconstruction electron microscopy

*Professor A.I. Kirkland*

We are developing numerical techniques for reconstructing exit-waves from crystals to enable us to extract both the amplitudes and phases of diffracted beams. In this way the useable information in lattice imaging from the JEOL 3000F instrument can be extended out as far as 1 angstom. In the case of complex oxide structures the positions of the oxygen atoms are clearly revealed by this technique.

## Control of quantum dot growth by sub-surface dislocations

*Professor D.J.H. Cockayne, C. Lang, Dr. D Nguyen-Manh*, Dr. F Ross***

The quantum dots (QDs) investigated in this work are nano-sized semiconductor islands which, due to their size, exhibit novel electronic properties. They take microelectronics to the next stage of nanoelectronics. QDs typically involve the growth of small islands of one semiconductor on another semiconductor acting as a substrate. For progress in this field, it is necessary to develop methods for the controlled growth of QDs, preferably in arrays. This project aims to study the effectiveness of dislocations embedded in crystalline substrates as nucleation sources for the growth of QDs, and specifically their effectiveness in controlling the composition and sizes of the QDs. This will be done in a combined theoretical and experimental study in collaboration between the University of Oxford, Culham Science Centre (UKAEA), and IBM (Yorktown Heights, USA). These three laboratories bring together a unique combination of materials characterisation, modelling and in-situ observation during QD growth. (*UKAEA, ** IBM USA)

## Aberration-corrected electron microscopy for high resolution analysis and imaging

*Professor D.J.H. Cockayne, Professor A.I. Kirkland, Dr. J.L. Hutchison, Dr. C.J.D. Hetherington, Dr. P.D. Nellist*

As part of a major research grant, the Department has secured funding which enables us to work closely with an electron microscope manufacturer in developing the next generation of high performance electron microscopes. The new instrument includes a field-emission-gun, two aberration correctors and various advanced detectors which provide analysis and spatial resolution capabilities at the 1 angstrom level. The instrument is being used for atomic-scale investigations of a range of new materials. (Funded by the Joint Infrastructure Fund)

## NanoSIMS analysis of metallic and electronic materials

*S. Ahmed, Dr. M. Schroder, Dr. S. Lozano-Perez, Professor C.R.M. Grovenor, Professor J.M. Titchmarsh*

A Cameca NanoSIMS50 has recently been installed at the Oxford University Begbroke Science Park. This equipment is a state-of-the-art machine for chemical analysis with high spatial resolution and very high sensitivity for most elements. We will use this new facility in projects where the accurate analysis of the distribution of dilute element is critical to developing a better understanding of the materials properties. Key projects include; [1] Crack and grain boundary chemistry in stainless steels (in collaboration with the Universities of Manchester and Birmingham and Johnson Matthey, and with INSS in Japan) [2] Trace element chemistry in structural steels (in collaboration with Corus) Funding provided by EPSRC for DTA studentship for SA.

## NanoSIMS analysis of Biological Materials

*K. Smart, G. Karney, K-H. Lau, Dr. M. Schroder, Professor C.R.M. Grovenor, Dr. J.T. Czernuszka*

A Cameca NanoSIMS50 has recently been installed at the Oxford University Begbroke Science Park. This is a state-of-the-art facility for chemical analysis with high spatial resolution and very high sensitivity for most elements. 50% of the time on this new facility is dedicated to studies of biological materials with support from the Life Science Inititative of the EPSRC under GR/T19797. Current projects include; [1] the localisation of metal complexes in a study of new imaging and therapeutic agents for hypoxic tissue (with Prof. J. Dilworth, Department of Chemistry). [2] Trace element localisation and isotopic analysis in teeth (with Dr A.Pike, Dept. Archaeology, University of Bristol and Prof. J.Elliot, QML) [3] Metal localisation in hyperaccumulator plants (with Professor Andrew Smith, Department of Plant Sciences) [4] SIMS analysis of the proteome of a single cell (with Profs. G.Misevic and C. Ripoll, Laboratoire "Assemblages Moléculaires: Modélisation et Imagerie SIMS" Faculté des Sciences de l'Université de Rouen)

## Remote Microscopy

*Professor D.J.H. Cockayne, Professor P. Jeffreys*, M. Dovey*, Professor A.I. Kirkland, D. Hutton, Dr. M. Rahman*

This project has developed a dedicated SEM for remote access over the WWW. It is being ""rolled out"" to schools from where it can be booked and operated on-line. Modules for use within the secondary school curricula have been developed and are being tested. In time, access will be given to museums and industry. (Funded by DTI and JEOL)

### 3-D microstructural analysis using a FIB system

*Professor J.M. Titchmarsh, Dr. B.J. Inkson*, Dr. G. Mobus**

A focused ion-beam system is being used to mil a set of cross-sections through a chosen area. The images obtained are being used to reconstruct the 3-dimensional microstructure. The suitability of this technique to a range of different systems and the errors associated with the milling and the 3-D reconstruction are being assessed.(Funded by the EPSRC)(*Department of Engineering Materials, University of Sheffield)

### Experimental and theoretical electron energy loss studies of carbon nanostructures

*Dr. R.J. Nicholls, Professor D.J.H. Cockayne, Professor A.I. Kirkland, Professor D.G. Pettifor, Professor G.A.D. Briggs*

The local density of unoccupied electronic states is of vital importance in quantum nanotechnology. A combination of experimental electron energy loss spectroscopy and density functional and multiple scattering theories is an ideal way in which to study these states. We are using this combination of experiment and theory to probe the electronic structure of carbon nanomaterials. The aim is to better understand the interaction between a nanotube and endohedral fullerenes encapsulated inside it. (Partly funded by DSTL)

### Interface Engineering of Multilayer Nanostructures

*Professor M. Bilek*, A/Professor D. McCulloch**, Professor D.J.H. Cockayne,*

Nanostructured multilayers can outperform coatings of their constituent layers in both hardness and strength. It is believed that the nature of interfaces in these materials is critical since they mediate dislocation motion and crack propagation. This project will use advanced synthesis, microanalysis and theoretical methods to investigate multilayer coatings with sharp, diffuse and rough interfaces in order to reveal their failure mechanisms under stress. This will enable us to understand the principles required to design the strongest structures and facilitate the selection of materials and deposition parameters in order to produce coatings optimised for a range of demanding applications (Funded by ARC) (University of Sydney*, RMIT**)

### Quantitative Atomic resolution Imaging

*Professor A.I. Kirkland*

Almost all structural information derived from High Resolution Electron Microscopy relies on qualitative matching of observed and calculated image contrast. This project aims to investigate the fundamental reasons as to why the calculated and measured intensities differ by significant amounts and to develop quantitative approaches to image matching.

### New Detectors for Transmission Electron Microscopy

*Professor A.I. Kirkland, Dr. P.R. Wilshaw, Dr. C.J.D. Hetherington*

Current generation imaging detectors for Transmission Electron Microscopy rely on a complex electron-photon conversion chain with the photons being detected by Charge Coupled Devices. As a result the overall sensitivity of these systems is poor and they are limited in their frame rate. We aim to construct the next generation of direct electron detector and this project will involve both computation and ultimately fabrication of a prototype device. (Funded by Leverhulme Trust)

### Novel Approaches to Direct Object Reconstruction in Transmission Electron Microscopy

*Professor A.I. Kirkland, Dr. C. Dwyer, Dr. L-Y. Chang*

All Transmission Electron Microscope Images are resolution limited by the aberrations of the objective lens. This project aims to develop novel approaches to overcoming these limitations through direct reconstruction from combinations of imaging and diffraction experiments capable of achieving sub Angstrom resolution.

### Aberration-corrected high resolution electron microscopy

*Professor A.I. Kirkland, Dr. J.L. Hutchison,*

We are exploring ways of adjusting spherical aberration in high resolution electron microscopy as a way of obtaining 0.1 nm resolution, and also as a way of controlling phase contrast, particularly in the study of nanocrystalline particles in the 1 - 2 nm size range.

## *TEM investigation of PRAM Materials and Devices*

*Professor D.J.H. Cockayne, Dr. Se Ahn Song*, Dr. C. Lang, Y. Chen*

The phase change memory device (PRAM) is considered as the next generation device which will compete with DRAM and Flash memory. Key materials for the PRAM are thin films such as Ge2Sb2Te5. These alloys can have a range of possible amorphous structures, but understanding of the structure of such thin films is not at all straightforward because of the small volumes of material available for analysis in PRAM systems. The radial distribution function technique using energy selected electron diffraction has been developed specifically to give the radial distribution function (RDF) of thin films like those to be investigated in this project. The interpretation of the RDF from alloys is, however, not straightforward, and studies of model systems are required to confidently interpret the data. This includes simulating the RDF from model structures and use of RMC techniques for refinement against the data. (*Samsung, Korea)

## *NanoSIMS analysis of early life on earth*

*Professor M. Brasier*, Dr. D. Wacey*, Dr. M. Schroder, Professor C.R.M. Grovenor*

Endolithic microborings in Archean sedimentary rocks provide important evidence of early life on Earth and beyond. They comprise small tubes (typically 10 microns in diameter) within siliceous chert, often infilled with Carbon and sulphur bearing minerals. The authenticity of such purported microfossils, however, depends on being able to establish a biogenic origin. Brazier et al in the Department of Earth Science have recently discovered a unique assemblage of <3520 Ma old mineralised microtubules from Western Australia. This is potentially the ""oldest"" example of life on Earth. We are using the Cameca NanoSIMS 50 to measure Carbon and Sulphur isotopic ratios in extremely small volumes to ascertain whether the mineral assemblages are indeed biogenic in origin. (Funded by NERC) (*Department of Earth Sciences)

## *Theory of Aberration Corrected Imaging*

*Professor A.I. Kirkland, Dr. L.Y. Chang*

This project will investigate the theory of imaging under aberration corrected imaging conditions using the recently installed double Cs aberration corrected TEM in the Department.

## *Fundamentals of Aberration Corrected Imaging in the TEM*

*Professor A.I. Kirkland*

The department has installed the world's first electron microscope with aberration correctors in both the condenser (probe-forming) and objective (image forming) lenses. This project aims to develop an understanding of the image contrast theory appropriate to this instrument, and to develop experimental techniques for exploiting variable aberration imaging. Possible materials candidates for experimental and theoretical studies include complex oxides and carbon nanotubes.

## *NanoSIMS analysis of biomineralisation processes in marine coccoliths*

*Dr. R. Rickaby*, Dr. M. Schroder, Professor C.R.M. Grovenor*

Palaeoclimates can be reconstructed using trace element ratios in the calcite skeletons of micro-marine organisms such as Coccolithophores and Foraminifera. These unicellular, calcifying oceanic phytoplankton, provide outstanding models for the analysis of the biomineralisation processes because they are robust, simple systems easy to culture in the laboratory. There are at least two steps during the biomineralisation process which must impact the calcite chemistry; the transport of ions from seawater across membranes to the site of precipitation within an intracellular vesicle, and the precipitation of calcite on an organic matrix. We are using the Cameca NanoSIMS 50 to study these processes in order to develop a better understanding of these key biomineralisation processes. (In collaboration with Dr. Alison Taylor and Prof. Colin Brownlee at the Marine Biological Association in Plymouth). (*Department of Earth Sciences) Funded by EPSRC.

## *A study of the column approximation in the kinematical theory of image contrast, and its effect on weak-beam imaging of defects*

*Professor Sir Peter Hirsch, Professor D.J.H. Cockayne, Dr. Z. Zhou*

The interpretation of diffraction contrast images often requires the support of image calculations and/or simulations. In many circumstances (e.g. weak beam images), the kinematical theory within the column approximation gives an intuitive and simple approach. Developments of this approach are being investigated.

### *Environmental cracking of stainless steels*

*Dr. S. Lozano-Perez, Professor C. English, Professor G.D.W. Smith*

Advanced characterisation techniques, including TEM, NanoSIMS and 3-D Atom Probe, are being used to investigate the mechanisms of stress corrosion cracking of austenitic stainless steels. The effect of prior cold work on the crack growth process is a particular focus of the research (Funded by INSS, the Institute of Nuclear Safety System, Japan).

### *Three-dimensional imaging and analysis through scanning confocal electron microscopy*

*Dr. P.D. Nellist, Professor A.I. Kirkland, E.C. Cosgriff, G. Behan, Professor L. Allen**

The department has installed the world's first electron microscope with aberration correctors in both the condenser (probe-forming) and objective (image forming) lenses. It is possible to use both lens systems together to form a confocal microscope, which allows atomic resolution imaging and analysis in two dimensions simultaneous with nanometre-scale resolution in the third dimension. We are attempting to apply this technique to a diverse range of materials from buried interfaces in semiconductor devices to screw dislocation core structures. (* University of Melbourne, Australia)

### *The atomic and electronic structure of inorganic nanowires*

*Dr. P.D. Nellist, Dr. V. Nicolosi*, Dr. J. Coleman*, Professor J. Boland*, Dr. J. Holmes***

Some molybdenum chalcogenide based compounds naturally grow as one-dimensional molecules, that can be seen to self-assemble into bundles with varying degrees of order. Other inorganic nanowires can be synthesized using mesoporous templates. It is only possible to characterize these wires using techniques with high spatial resolution, and we are applying scanning transmission electron microscope techniques such as Z-contrast imaging and electron energy-loss spectroscopy in order to measure their atomic and electronic structure. Using an aberration-corrected STEM has revealed unexpected structures and assembly processes, and we are investigating methods to observe the assembly in the microscope. (*Trinity College Dublin, Ireland; **University College Cork, Ireland)

### *Quantitative interpretation of aberration-corrected STEM data*

*Dr. P.D. Nellist, E.C. Cosgriff*

The development of aberration-correctors for the STEM has led to a dramatic improvement in lateral spatial resolution along with a reduction in the depth of focus. Making quantitative interpretation of these data requires a complete understanding of the electron scattering mechanisms under these illumination conditions. Using simulations and theory we are building our understanding of the scattering mechanisms which will allow enhanced use of the powerful new data sets that we can now record.

### *Weak-beam TEM of end-on images of screw dislocations*

*Dr. Z. Zhou, Professor D.J.H. Cockayne, Professor Sir Peter Hirsch*

Diffraction contrast from end-on images of screw dislocations is caused by surface relaxation displacements. The theory of weak-beam image contrast due to these displacements is being developed fro dislocations in thin foils. The contrast is in the form of bright and dark lobes on opposite sides of the dislocation. The sense of this asymmetry depends on the size of the burgers vector. A joint project is being formed with Professor Y. Ikuhara (Institute of Engineering Innovation, Tokyo University) and Dr. A Nakamura (Department of Materials, Osaka City University) to apply this technique to determine the signs of the screw components of the Burgers vectors in end-on images of grain boundary dislocations in alumina.

### *Can the predicted edge components fo the core structure of screw dislocations in Mo be imaged by HREM?*

*Dr. Z. Zhou, Professor D.J.H. Cockayne, Professor Sir Peter Hirsch*

The surface relation strains around screw dislocations normal to thin foils affect the core structure near the surface. Professor Vitek's group (University of Pensylvania) have calculated the magnitude of the effect for Mo, and Professor Hemker and his group (Department of Mechanical Engineering, John Hopkins University) are using these data to calculate the HREM images to see whether the images reflect the core structure in an infinite crystal, or that near the surface.

# IV - RADIATION DAMAGE

## Mechanisms of embrittlement in reactor pressure vessel steels

*Dr. M.L. Jenkins, Professor J.M. Titchmarsh, Dr. S. Lozano-Perez*

Electron microscopy of heat - treated and irradiated pressure vessel steels and model alloys is being carried out to identify the mechanisms by which these materials become embrittled during neutron irradiation, with particular emphasis on (i)the precipitation of copper-rich particles, and (ii)identification of the matrix component of hardening. Methods used include high-resolution electron microscopy, EELS mapping and in-situ straining. (Funded by EPSRC and Rolls-Royce)

## TEM studies of radiation damage in materials for fusion reactors

*Dr. M.L. Jenkins, Dr. S.G. Roberts, Dr. Z. Yao, Sen Xu, Dr. M.A. Kirk**

Materials issues will be crucial to the success of future fusion reactors. Structural materials will operate at temperatures up to 600C, will need to withstand stresses up to 300MPa, and will accumulate over their lifetime radiation damage from fast neutrons amounting to ~100 displacements per atom, combined with high levels of helium and hydrogen produced in transmutation reactions. It is essential that any material used maintains adequate strength and toughness, while suffering minimal dimensional changes through swelling and creep. Candidate materials include ferritic/martensitic steels based on iron ~9% chromium, ODS steels, vanadium alloys and tungsten. This project uses advanced techniques in electron microscopy to characterise the development of radiation damage in these materials and in model FeCr alloys. We perform both high-energy (MeV) ion irradiations of bulk materials and in-situ heavy-ion irradiations in the Argonne IVEM-Tandem Facility. We work closely with the materials modelling group who are applying multiscale modelling techniques to the same materials. (Funded and in collaboration with EURATOM/UKAEA, *Argonne National Laboratory)

## Characterisation of defect clusters using elastic diffuse scattering patterns and energy-filtered images

*Dr. M.L Jenkins, Professor A.P. Sutton*, Dr. Z. Zhou, Dr. S.L. Dudarev**, Dr. M.A. Kirk****

New electron-microscope characterisation techniques based on energy-filtered imaging and diffraction are being developed. A particularly promising new technique (developed by Kirk) involves measurements of elastic diffuse scattering near weakly excited diffraction peaks from isolated small point-defect clusters. The asymmetry in the diffuse scattering immediately reveals the interstitial or vacancy nature of the cluster. This technique is now being explored systematically, including simulations of elastic diffuse scattering patterns. (*Imperial College, **EURATOM/UKAEA, *** Argonne National Laboratory)

## Electron microscope image simulations under weak-beam diffraction conditions

*Dr. M.L. Jenkins, Dr Z. Zhou*, Professor A.P. Sutton**, Dr. M.A. Kirk***, Dr. S.L. Dudarev*****

This project is focused on the development of a new approach to the interpretation of electron microscope images of small point defect clusters and dislocations. The approach is based on the theory developed by Howie and Basinski, where quantum interference between non-parallel diffracted electron beams is taken into account. We have developed a computer code implementing the Howie and Basinski equations, to allow image simulations under weak-beam and dynamical contrast conditions of dislocation loops, SFT and eventually nanoclusters of complex morphology. These image simulations will be matched with experimental images of small clusters produced by radiation damage of metals. (*Cardiff University, **Imperial College, ***Argonne National Laboratory, ****EURATOM/UKAEA)

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# G. Modelling and Simulation

A materials modelling laboratory was set up in 1992 on the top floor of 21 Banbury Road. It currently houses a suite of Hewlett-Packard, Silicon Graphics and LinuxPC workstations. The laboratory acts as the focus for all computational modelling within the Department of Materials. It is a world-leading facility in that the research spans the entire spectrum from quantum mechanical atomistic simulations through the microscopic scale to macroscopic continuum modelling. The work of the laboratory supports and complements the in house experimental programmes and has close links with industry.

## *Organic light emitting diodes incorporating quantum dots*

*Dr. K. Kohary, Dr. V.M. Burlakov, Professor D.G. Pettifor, G. Gibson*, C. Nauka*, C.C. Yang*, Dr. J. Brug**

Inorganic nanocrystal quantum dots incorporated into organic light emitting diodes (OLEDs) have been suggested as a new form for solid-state lighting. This hybrid device exploits the large variety of potential applications of organic materials combined with the high performance electronic and optical properties of inorganic nanocrystal quantum dots. In this project we perform a theoretical analysis of the efficiency of OLEDs activated by nanocrystal quantum dots embedded between hole and electron transport layers of organic semiconductors. Assuming diffusion controlled charge transport in the organic media, we study the formation of excitons and their injection into the quantum dots via the Forster exchange mechanism. We also include exciton formation within the quantum dots via direct charge injection. (*Hewlett-Packard Laboratories, Palo Alto, California).

## *MBE growth of spintronic materials*

*Professor D.G. Pettifor, Dr. R. Drautz, D. Murdick*, B. Gillespie* Dr. X. Zhou*, Professor H. Wadley**

Analytic bond-order potentials (BOPs) are being developed for modelling the MBE growth of spintronic materials such as Mn in GaAs films. (*University of Virginia) (Funded by DARPA).

## *First principle studies of intermetallics*

*H.R. Chauke*, M. Phasha*, Professor P.E. Ngoepe*, Dr. R. Drautz, Dr. D. Nguyen Manh**, Professor D.G. Pettifor*

The electronic structure, equation of state and phase stability of platinum aluminides and magnesium-lithium alloys are being predicted using first principles density functional theory. (*Materials Modelling Centre, University of the North, South Africa; **UKAEA, Culham) (Funded by Royal Society - FRD collaborative project)

## *Modelling photo-induced changes during growth of amorphous chalcogenide films*

*Dr. K. Kohary, Professor D.G. Pettifor, Professor S. Kugler**

The photo-induced volume changes in amorphous chalcogenide semiconductors will be modelled using a tight-binding molecular dynamics scheme in order to analyse the bond-breaking mechanisms responsible for the photo-induced instabilities. (*Budapest University of Technology and Economics.) (Funded by British Council).

## *Molecular dynamics models of thermally activated mobility of dislocations in dilute bcc alloys*

*M.R. Gilbert, Dr. S.L. Dudarev*, Professor D.G. Pettifor*

Alloy softening of several bcc metals occurs for a range of alloying additions and is believed to be associated with the "catalytic" effect of the solute atoms on the thermally activated propagation of dislocations. This will be investigated using large-scale molecular dynamics simulations. (*UKAEA Culham). (Funded by UKAEA Culham).

## *Development of analytic bond-order potentials for magnetic transition metals*

*Dr. R. Drautz, Professor D.G. Pettifor*

Analytic bond-order potentials for magnetic bcc transition metals and alloys such as the ferritic-martensitic steels will be developed and applied to modelling defect behaviour within the EPSRC-funded modelling consortium on 'Modelling of materials for fusion reactors'. (Funded by EPSRC).

## *Modelling the growth of carbon nanotubes*

*K. Zhang, Dr. R. Drautz, Dr. N. Grobert*

Analytic bond-order potentials and molecular dynamics are used to model the growth of carbon nanotubes. This projects links in directly with growth experiments and high resolution electron microscopy studies of carbon nanotube materials within the Department.

## *Theory and Modelling of Nano-morphology*

*Dr. A.S. Barnard*

A new shape-dependent model is in development, capable of describing the thermodynamics of arbitrary quasi-zero dimensional nanocrystals (including quantum dots), and quasi-one dimensional structures (nanorods and nanowires) with either simple or complicated polyhedral shapes. The model takes as input parameters calculated from first principles and is applicable at sizes traditionally inaccessible to ab initio methods (between approximately 3-100 nm in diameter). Using this model it is possible to investigate the equilibrium shape of nanomaterials as a function of a number of experimentally relevant parameters such as size, temperature, surface chemistry or chemical potential. Recent advances include additional terms to describe planar defects, thereby allowing the modelling of twinned and decahedral structures. One of the aims of this program is to provide a framework for comparing the phase stability of polymorphs as a function of shape (and to create shape-phase diagrams), as well as facilitating comparison of the relative stability of non-equilibrium shapes under desired conditions. (Supported by The Glasstone Trust)

## *Modelling brittle-ductile transitions in BCC metals for fusion power applications*

*E. Tarleton, Dr. R. Novokshanov, Dr. A.J. Wilkinson, Dr. S.G. Roberts*

The project investigates the effects of radiation on mechanical properties, especially the brittle-to-ductile transition, in vanadium, tungsten and iron-chromium alloys. 2-D and 3-D dislocation dynamic models will be developed to simulate the interaction of radiation damage with dislocation motion and the effects on yield, flow and fracture behaviour. (Funded by EPSRC)

## *Modelling the yield stress and brittle-ductile transition in silicon deformed in 3-point bending*

*Dr. S.G. Roberts, Professor Sir Peter Hirsch*

Experiments by Folk (2000) on deforming initially dislocation-free Si by 3-point bending formed a brittle-ductile transition above a critical temperature Tc. Below Tc the specimens fail by brittle fracture, preceded by limited plasticity. A simulation has been carried out, based on a simple model, which explores quantitatively the dependence of the upper yield point and fracture stress on temperature and strain-rate, and that of Tc on strain rate. The critical flaws for brittle fracture are identified as steps or notches produced by slip-lines on the tensile surface.

## *Stability of Intergranular Films at Grain Boundaries in Silicon Nitride*

*Dr. C.M. Bishop, Dr. R.M. Cannon*, Professor W.C. Carter***

General grain boundaries in silicon nitride exhibit intergranular glassy films. The goal of the project is to apply a diffuse-interface theory for interfaces in multi-component, complex materials to silicon nitride in order to understand the effects that stabilise intergranular films.(*Lawrence Berkeley National Laboratory, Berkeley, USA, ** Massachusetts Institute of Technology, Cambridge, USA)

## *Tuning Phase-Field Models with Experimental Data*

*Dr. C.M. Bishop, Dr. C. Koch**

Phase-field models of complex materials contain empirical parameters that are non-trivially related to interfacial energies and interfacial widths by different measures. The goal of this project is to develop methods for fitting the empirical parameters to information derived from electron microscopy. (*Max-Plank Institut fur Metallforschung, Stuttgart, Germany)

## *Shape and Phase Stability of Colloidal Oxide Nanoparticles*

*Dr. H. Xu*, Dr. A.S. Barnard*

In recent years it has been found that many colloidal nanoparticles exhibit a reversal of phase stability with respect to the bulk analogues. In addition to this, the same colloidal nanoparticles may form in a variety of different shapes, depending in part upon the size and phase. Examples include the tetragonal and monoclinic polymorphs of zirconium dioxide, and the anatase and rutile polymorphs of titanium dioxide. This project uses thermodynamic modeling and first principles computer simulations to investigate the role of nanomorphology in affecting the size-dependent phase transition in oxide nanoparticles, and understand the intrinsic link between the free energy of formation and the prevalence of particular surface facets. From these results it becomes apparent that variations in the thermochemical results reported in the literature may also be partially attributed to variations in nanocrystal shapes. (*Department of Geology & Geophysics and Materials Science Program, The University of Wisconsin, Madison, WI, USA) (Supported by the Glasstone Trust, the National Science Foundation and the Graduate School of the University of Wisconsin - Madison.)

### *Modelling the formation of hydrogen-bonded molecular networks on crystalline surfaces*

*U. Weber, Dr. V. Burlakov, Professor D.G. Pettifor, Professor J.H. Jefferson*, Professor G.A.D. Briggs*

The main objective is to develop a model suitable for simulation of hydrogen-bonded molecular networks on crystalline surfaces taking into account a mismatch between the crystal structures of the surfaces and the molecular network. An important part of the project is related to the development of environment-dependent potential describing hydrogen bonds between the network-forming molecules. This potential will then be used in kinetic MC simulations to guide experimental studies of the molecular networks and the structures suitable for QIP on different substrates. The potential parameters will be extracted using ab initio calculations performed in collaboration with L. Kantorovich (King's College, London), and verified against experimental studies carried out in the groups of P. Beton and N. Champness (Nottingham University). (*QinetiQ).(Funded by EPSRC).

### *Modelling supramolecular assembly on surfaces*

*Dr. V. Burlakov, Professor D.G. Pettifor, Professor J.H. Jefferson*, Professor G.A.D. Briggs*

The aim of the project is to understand the formation and stability of hydrogen-bonded molecular networks on crystal surfaces. The key parameters are related to intermolecular binding energies, molecular adhesion to the surfaces, and commensurability of the network with the underlying lattice. Formation of the networks is being modelled using the kinetic Monte Carlo technique. The model parameters, such as molecular diffusion coefficients, are going to be calculated ab initio in collaboration with L. Kantorovich (King's College, London), and compared with the experimental studies carried in the groups of P. Beton and N. Champness (Nottingham University). (*QinetiQ).(Funded by EPSRC).

### *Structure, Shape and Phase Stability of Boron Nitride Nanomaterials*

*Professor S.P. Russo*, Professor I.K. Snook*, Dr. A.S. Barnard*

This project uses density functional theory to investigate the bonding, structure and phase stability of the zinc-blende (fcc), wurtzite (hcp) and hexagonal polymorphs of boron nitride at the nanoscale. The role of shape, curvature and stoichiometry (defects) in moderating formation energies are of particular interest. (*Applied Physics, RMIT University, Melbourne, AUST) (Supported by the Glasstone Trust)

### *Shape and Structure of Gold Nanoparticles*

*Dr. L.A. Curtiss*, Dr. A.S. Barnard*

This project used thermodynamic modeling and relativistic density functional theory computer simulations to investigate the relationship between size, shape, structure and temperature of colloidal gold nanoparticles. Both fcc (or different shapes) and quasi-crystalline structures are considered - with and withour alkane-thiol surfactants. (* Materials Science and Chemistry Divisions, Argonne National Laboratory) (Supported by the Glasstone Trust, and the U.S. Department of Energy, Basic Energy Sciences, under contract W-31-109-ENG-38.)

### *Alloys by design: application to Ni-based superalloy turbine blades*

*Dr. T. Hammerschmidt, Dr. R. Drautz, Professor D.G. Pettifor*

Atomistic simulations are employed to characterize the thermodynamic and kinetic stability of superalloy phases and their interfaces using analytical bond-order potentials. Of particular interest are the influence of alloying components such as Mo, Re, Ru on the stability of detrimental topologically close packed phases such as sigma, mu, P and R. (In collaboration with Imperial College London and the University of Cambridge. Funded by EPSRC).

### *Development of analytic bond-order potentials for bcc transition metals*

*T. Qin, Dr. R. Drautz, Professor D.G. Pettifor*

Analytic bond-order potentials for non-magnetic bcc transition metals such as V and W will be developed and applied to modelling defect behaviour within the EPSRC-funded modelling consortium on 'Modelling of materials for fusion reactors'. (Funded by EPSRC).

### *Modelling damage evolution in fusion reactor materials*

*N. Aggarwal, Dr. R. Drautz, Professor S.G. Roberts*

The evolution of radiation-induced defects in bcc metals beyond the molecular dynamics timescale is being modelled using kinetic Monte-Carlo. The project will provide information about densities of defects, as well as the dominant types of defects, at various stages of microstructural evolution. This information will be used by collaborating researchers in modelling plastic deformation and fracture. (Funded by EPSRC). t

# H. Materials Science Based Archaeology

The Materials Science Based Archaeology Group is concerned with the investigation of all aspects of the metallurgical process, from smelting to metal finishing, and from the first use of alloys in the 5th/4th millennia BC to the Industrial Revolution. The themes of the research can be broadly labelled as archaeological and metallurgical. In archaeology the research derives from post-excavation and museum-based projects involving the characterization of the products and residues of past metallurgical processes. The results are used to explore the place of metals in ancient economies and societies, how they were made, used, traded and re-cycled, how their properties were understood, and what processes were associated with their deposition and survival in the archaeological record. This work is supported by experiments designed to relate this material to the process variables which shaped its formation. These experiments also form a link with the metallurgical objectives of the group. These are to acquire a deep knowledge of the physical and mechanical metallurgy of the metals used in the past, so that we can see how they were understood in the past. The results can be surprising and demand novel research, for example to determine why some alloys have an exceptional ductility. This work also links directly with other areas of metallurgy by extending to 6x103 years the time range available for studying a variety of room temperature phenomena from corrosion to precipitation, and with results applicable in such diverse fields as electronic packaging and the storage of nuclear waste.

### *Non-ferrous metallurgy in the European Iron Age*

*Dr. J.P. Northover, P. Nagy*, P. Ramsl***

The study of bronze objects from Iron Age cemeteries, settlements and hoards in Austria, Denmark and Switzerland is showing how copper-based metallurgy changed when bronze ceased to be the main utilitarian metal. Attention is presently focussed on cemeteries to look for associations between gender, status and ethnicity of individuals and the technical quality and origins of the objects buried with them. (*Kantonsarchäologie Zürich; **Naturhistorisches Museum, Wien)

### *The study of thick corrosion layers on archaeological metals using controlled laser ablation in conjunction with an external beam microprobe*

*M.H. Abraham, Dr. G.W. Grime*, Dr. J.P. Northover*

The variation with depth of the composition of corrosion layers on buried metal objects can provide the archaeologist with valuable information relating to the burial conditions of the object. In some cases these layers can be very thick (exceeding 1mm) so normally destructive methods such as sectioning are used to characterise the layers. The technique developed here uses a micro-focussed high power pulsed Nd-YAG laser to ablate the corrosion layer in a series of controlled steps, while monitoring the composition of the exposed surface using PIXE and RBS in the external beam facility of the scanning proton microprobe.. Thus important information about the composition, condition and history of an object can be recovered with minimal physical intervention. (*University of Surrey)

### *Early metallurgy in the Upper Euphrates Basin*

*Dr. J.P. Northover, Dr. K. Prag**

Microanalysis and metallography have been used to characterise the metalwork from a number of major excavations in the upper Euphrates basin. The sites straddle political and economic boundaries of the 3rd millennium BC during the period when bronze became the main utilitarian metal. The results have given us a new understanding of the way in which bronze became part of the metal economy and have also directed our attention to the importance of recycling in these early cities. (*University of Manchester).

### *Application of the scanning proton microprobe to the analysis of ancient bronze*

*M.H. Abraham, Dr. G.W. Grime*, Dr. J.P. Northover*

The requirements of museum collections have stimulated this project in non-destructive and minimally destructive analysis of ancient bronze. The project uses a laser to mill sub-millimetre diameter windows in the patina of selected bronzes and then use the scanning proton microprobe to analyse the metal as it is exposed, with the X-ray and RBS mapping facilities employed to make basic metallographic observations. The project is optimising the operation of the instrument in this mode and assesses the quality of the data in relation to sample-based analysis and microscopy. (*University of Surrey)

## *Study of the products of the experimental reproduction of the iron-working process at Bryn Y Castell and Crawcwellt Sites, Gwynedd*

*C.J. Salter, P. Crew**

A series of iron smelting and smithing experiments have been carried out to reproduce the metal and other iron-working debris from these important Iron Age sites. Presently, this material is being studied, an attempt to fully understand the chemistry, microstructure and mechanical properties of the different types of iron and steel produced. (*Snowdonia National Park Study Centre, Maentwrog, Gwynedd)

## *Copper extraction at Ross Island, Co. Kerry, Ireland*

*C.J. Salter, Dr. W. O'Brien**

A project to characterise copper and associated residues produced from the earliest copper mine in Ireland, dating to the second half of the third millennium BC. (*National University of Ireland, Galway)

## *The characterisation of Islamic steels*

*Dr. B.J. Gilmour, C.J. Salter, Dr. J. Allan**

A long-term project to develop the characterisation of high carbon and alloy steels from the medieval Islamic world using a range of metallographic and microprobe techniques. (*Department of Eastern Art, Ashmolean Museum)

## *Metalwork of the Bronze Age-Iron Age transition in Britain*

*D. Bruns*, Dr. J.P. Northover*

Combining archaeological and metallurgical methods to understand the metalwork and metalworking in Britain at the time of the first introduction of iron in the 9th-7th centuries BC. This is the first ever systematic survey of the metalwork of this period and is leading to a new understanding of the chronology of the period and the quantity and range of the metalwork. (*Institute of Archaeology, Oxford University)

## *Medieval Islamic mint technology*

*Dr. J.P. Northover, L. Treadwell**

In the 10th-12th centuries CE the silver coinage of the Islamic Middle East and Central Asia shows a remarkable variety of combinations of alloy type and mint technology. This project, through detailed microstructural and compositional analysis will begin to characterise this variety and develop Â“family treesÂ” for their evolution. (*Ashmolean Museum).

## *Engineering metallurgy of the 18th and 19th centuries*

*Dr. J.P. Northover*

The engineering of the industrial revolution was constrained by the lack of bulk high strength structural materials, e.g. steel, and by the quality of the available basic materials, notably copper and wrought iron. Continuing research is using surviving material to determine the composition, structure and mechanical properties of copper and wrought iron and their alloys. Associated with this is a study of contemporary documents to show how material properties were understood, measured and described.

## *The Bronze Age metallurgy of Norway*

*Dr J.P. Northover, Dr A.-L. Melheim**

A pilot project for the first-ever full survey of the metalwork and metallurgy of the Bronze Age in Norway. (*University of Oslo)

## *Bronze Age Copper Ingots*

*Dr. J.P. Northover*

Analysis of Bronze Age copper ingots from Cornwall in conjunction with the Royal Cornwall Museum is leading to new understandings of the place ingots played in the circulation of metal and the distances over which copper was transported.

## *Investigation of the changes in metal and slag inclusion compositions during fire welding.*

*C.J. Salter, Dr. B.J.J. Gilmour*

A study of the changes in metal and slag inclusion compositions that occur during the forge welding of iron. In particular those changes seen in a variety of Anglo-Saxon phosphoritic/non-phosphoritic composite iron artefacts.

# *I. Third Leg and Other Projects*

## *Faraday Advance*

*Professor. P.S. Grant, Dr. C. Johnston, Dr. R.M.K. Young et al.*

Faraday Advance was established in February 2001 to act as a focus for future lightweight and high temperature materials for low pollution, high efficiency transport. New materials, their manufacturing technologies and their integration into engineering systems are critical if UK aerospace and automotive sectors are to meet global technical drivers. Faraday Advance's vision is to enable UK aerospace and automotive businesses to meet these requirements through a high quality, targeted and imaginative continuum of scientific and technical products and services. Faraday Advance focuses on six key technical drivers for the automotive and aerospace sectors: Â¥ Lightweight materials Â¥ Reduced emissions Â¥ End of vehicle life technologies Â¥ The powered or blended wing Â¥ The environmentally friendly aeroengine Â¥ More electric technologies

## *Oxford Centre for Advanced Materials and Composites (OCAMAC)*

*Dr. R.I. Todd*

The Oxford Centre for Advanced Materials and Composites (OCAMAC) is sponsored by the Departments of Materials, Engineering, Chemistry and Physics at Oxford University. The objective of OCAMAC is to foster interdisciplinary research into the scientific and technological problem of processing, properties, design and fabrication associated with advanced materials. OCAMAC aims to unlock research potential across sponsoring and other University Departments by stimulating research activity within the University and with industry, to disseminate results of research to the national and international materials community, and to deliver integrated technical solutions to industry.

## *Oxford Materials Charaterisation Services*

*Dr. A. Crossley*

Oxford Materials Characterisation Service (OMCS) deals with the commercial services offered by the Department of Materials. A dedicated team of experts provide fast and reliable turnaround of confidential and quality assured services, including: ¥ Consultancy with access to expertise within the Department of Materials ¥ Materials analysis and problem solving ¥ Training and access to state-of-the-art equipment

## *BegbrokeNano*

*Dr. A. Crossley, Dr C Johnston, Professor C.R.M. Grovenor, et al.*

BegbrokeNano, operated since 2005 by OMCS at Begbroke Science Park, is one of the UK Micro Nano Technology (MNT) Centres of Excellence funded by the DTI to provide cost effective open access facilities to organisations to accelerate commercialisation of MNT. BegbrokeNano, in partnership with leading analytical equipment manufacturers offers characterisation of products and processes at the micro and nano scale.

## *NANOSAFE II*

*Dr. M. Ratoi, Dr. J.A.A. Crossley, Professor P.J. Dobson**

NANOSAFE II ( www.nanosafe.org ) was established to explore concerns about the health, safety and environmental impacts of nanomaterials, as the use of nanotechnology applications and products increases. Its aim is to identify areas that could lead to potential health and environmental effects, establish research programmes by linking 24 research groups from 7 European countries together and stimulate the development of risk assessment and management protocols. Funded by the EC. (*Director of the University of Oxford Begbroke Science Park)

## *Smart Composites: EPSRC/Smiths Strategic Partnership*

*Professor P.S. Grant, Dr. S.R. Duncan**

EPSRC and Smiths have established jointly a 5 year Strategic Partnership with Oxford and Bristol Universities, in the area of smart composites. The focus for the research concerns two themes: (i) low cost manufacture of advanced structural composites; and (ii) novel embedded actuation materials and the associated systems technology. The research at Oxford concentrates on (1) the processing of smart composites; (2) the characterisation of their microstructure including actuation materials, interfacial properties and lifetime behaviour; and (3) modelling and control of actuation.

## *HITEN*

*Dr. C. Johnston*

HITEN is a global network of organisations interested in high temperature electronics (HTE). HITEN organise a biannual conference in Europe and publish current research, market and technology updates on all aspects of HTE. The main industrial sectors served by HITEN are well logging (geothermal and oil & gas), aerospace and automotive. High temperature electronics are defined as electronics operating in ambients above 125C.

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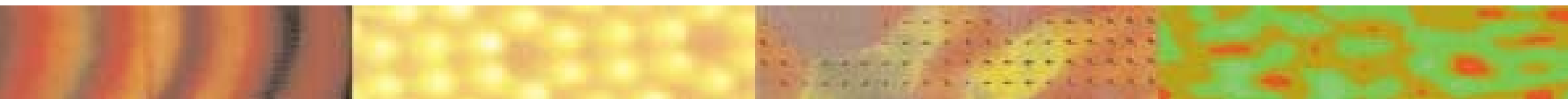

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