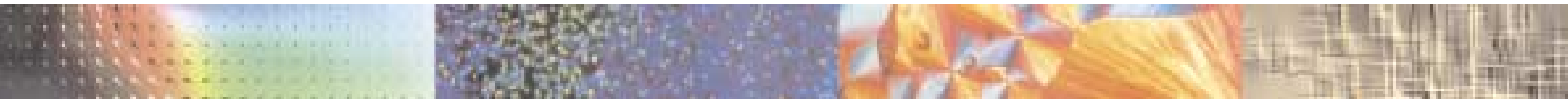
Oxford Materials

Research in Progress

2005 - 2006



Department of Materials

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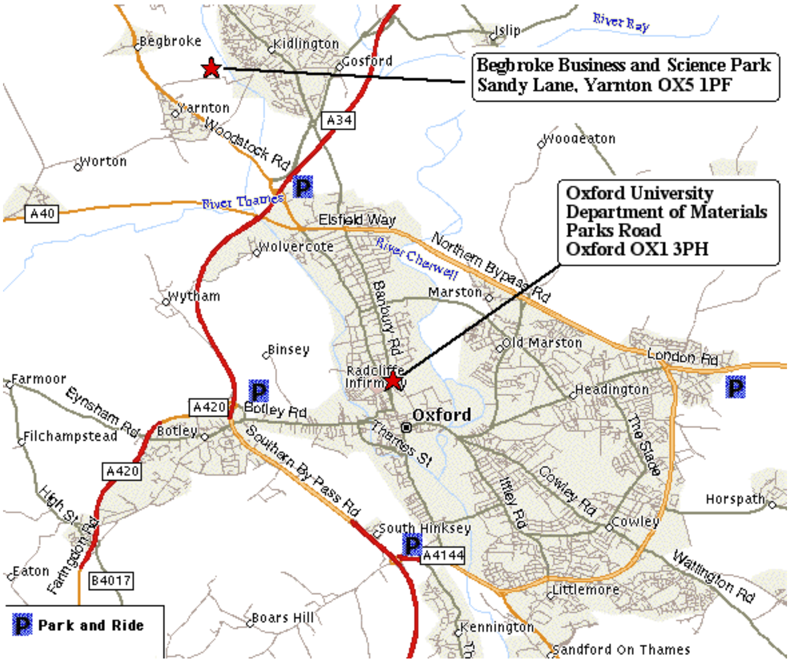
University of Oxford



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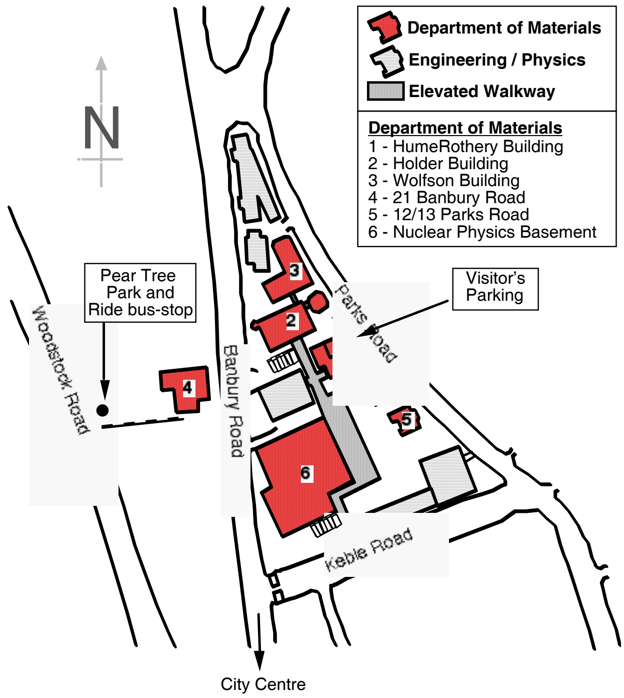
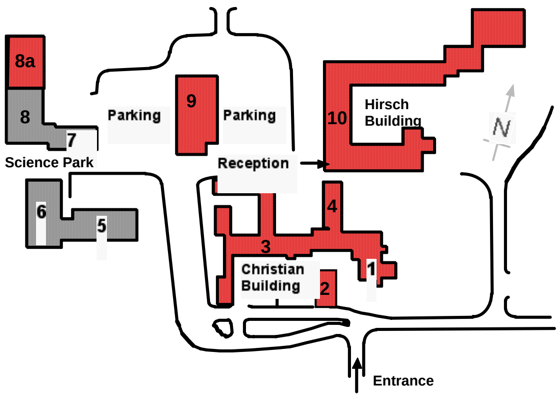


Begbroke Business and Science Park



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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 21 academics, 29 senior researchers, 40 postdoctoral researchers, 38 technicians and administrative staff, 64 academic visitors, and about 80 research students and 104 undergraduates. The Department is part of an integrated Division of Mathematical and Physical 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), the Acta Materialia Gold Medal (George Smith), the Beilby Medal and Prize (Alfred Cerezo), the Pfeil Award (Richard Todd), 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 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. 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. Four promotions to personal professorships (Adrian Sutton, Amanda Petford-Long, Alfred Cerezo and Chris Grovenor) and four promotions to readerships (John Hutchison, Mike Jenkins, Steve Roberts 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 £22m 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 designation of the Department as the main hub for 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 2005

Members of Department

Professors

Professor C.R.M. Grovenor	*Head of Department*
Professor D.G. Pettifor, FRS	*Isaac Wolfson Professor of Metallurgy* *Director of the Materials Modelling Laboratory*
Professor P.S. Grant	*Cookson Professor of Materials* *Director of Faraday Advance*
Professor D.J.H. Cockayne, FRS	*Professor in Physical Examination of Materials*
Professor G.A.D. Briggs	*Professor of Nanomaterials* *Quantum Information Processing Interdisciplinary Research Collaboration*
Professor A. Cerezo	*Professor of Materials*
Professor A.I. Kirkland	*Professor of 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. S.G. Roberts	*Reader in Materials*
Dr. J.M. Sykes	*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. K.A.Q. O'Reilly	*Lecturer in Materials*
Dr. J.M. Smith	*Lecturer in Materials*
Dr. R.I. Todd	*Lecturer in Materials* *Director of Oxford Centre for Advanced Materials and Composites*
Dr. P.R. Wilshaw	*Lecturer in Materials*
Dr. A.J. Wilkinson	*Lecturer in Materials*
Dr. D.G. Bucknall	*Visiting Lecturer in Materials*

Career Development Fellows

Dr. C. Bishop	*Career Development Fellow*
Dr. M. Galano	*Career Development Fellow*

Administration

Ms A. Davies	*Administrator*
Mr T. McAree	*Deputy Administrator (Finance)*
Dr. L.J.F. Jones	*Deputy Administrator (Academic)*
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. 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. N. Grobert	RS Dorothy Hodgkin 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. J.W. Martin	OCAMAC Senior Fellow
Dr. Duc Nguyen-Manh	OCAMAC Industrial Fellow (UKAEA)
Dr. C. Nörenberg	RS Dorothy Hodgkin Fellow
Dr. P.J. Northover	Senior Research Fellow
Dr. J. Sloan	Royal Society Research Fellow
Dr. S.C. Speller	RAE Research Fellow
Dr. I.C. Stone	Senior Research Fellow
Professor M. Stoneham	Senior Research Fellow
Dr. G. Taylor	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)

Research Fellows

Dr. D.E. Browne
Dr. V. Burlakov
Dr. A.M. Cock
Mr. F. Cullen
Mr. R.C. Doole
Dr. C. Dwyer
Dr. A. Gianattasio
Mr. T.J. Godfrey
Dr. B.M. Henry
Dr. C.J.D. Hetherington
Dr. S.C. Hogg
Dr. Y. Huang
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Dr. S. Lozano-Perez
Dr. J. Mercer-Lynch
Dr. J. Mi
Dr. R. Novokshanov
Dr. K. Porfyrakis
Dr. E. Sachlos
Mr. C.J. Salter
Dr. M. Sambrook
Dr. S. Senkader
Dr. G. Sha
Dr. H. Smith
Dr. T. Starke
Dr. M. Tanaka
Dr. J. Topping
Dr. J. Wallace
Dr. P.J. Warren
Dr. G.B. Winkelman
Dr. Z. Yao
Dr. C-Y. You
Dr. R.M.K. Young

D.Phil and MSc. Research Students

Abraham, M.H. (self-supporting)
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)
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)
Dancer, C. (EPSRC DTA)
Danvirutai, P. (Thai Gov.)
Dark, C.J. (EPSRC DTA)
Davidson, I. (CASE: Alcoa Extrusions)
Deak, D. (EPSRC)
Eggeman, A. (EPSRC DTA + CASE: Johnson Matthey)
Fitzsimons, J. (Helmore / EPSRC DTA)
Fraser. K. (EPSRC DTA)

Galano, M. (EU/Korea/Clarendon/ORS)
Ge, L. (Clarendon)
Gilbert, M. (UKAEA)
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)
Joseph, T. (CASE: UKAEA)
Karney, G. (EPSRC DTA)
Kawata, K. (Toppan Printing Co.)
King, O. (EPSRC)
Kirk, D. (EPSRC)
Kolli, A. (QIP IRC)
Korsah, M. (EPSRC)
Kumar, A. (EPSRC)
Lambourne, A. (Department)
Limpichaipanit, A. (Thai Gov.)
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
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.)
Porcu, M. (EPSRC DTA / EU)
Qin, T. (EPSRC)
Russell, B. (EPSRC DTA)
Rust, M. (NSF/Clarendon/ORS)
Saran, M. (Perdana Exchange Programme)
Shapiro, I. (EPSRC DTA)
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.)
Stowe, D.J. (EPSRC)
Tarleton, E. (EPSRC)
Thomas, G. (CASE: UKAEA)
Tiwari, A. (Clarendon)
Todorovic, M. (Scatchered Scholarship)
Tyrrell, E. (EPSRC DTA)
Vlandas, A. (EPSRC, St Cross College)
Wahl, D. (EPSRC)
Waller, J. (EPSRC)
Walpole, A. (EPSRC DTA)
Wang, C. (EPSRC)
Wang, H. (Clarendon/ORS)
Waring, M. (EPSRC DTA)
Whyte, E. (CASE:Corus)
Womersley, H. (EPSRC)
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)
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)

<u>Materials Science</u>
Barnes, D.H.
Gomberg, A.R.
Hardyment, A.
Hitchman, R.D.
Holden, M.F.B.
Holmes, S.R.
Jordan, D.M.
Lewis, P.J.
Lim, T.Y.C.
MacBride, J
McGhee, R.D.W.
Minshull, J.P.
Pickthorn, T.W.
Randman, D.
Taylor, J.M.
Wilkinson, C.M.F.
Williams, T.R.
Yao, Q.

<u>Materials, Economics and Management</u>
Aitio, A.E.U.
Bosworth, C.F.C.
Crofton, A-L.M.
Mittermaier, M.M.H.
Walker, A.N.
Wildy, S.

<u>Engineering and Material Science</u>
Barnard, J.
Curtis, A.
Kay, A.L.

Secretarial and Technical Support

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(Mr. A.B. Bailey)
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Mr. R. East
Mr. B.J. Fellows
Mrs. K. Fewings
(Mr P. Flaxman)
Mrs. P. Gordon
Mrs. K. Hartwell
Mr. M. Jackson
Mrs. L. Jenkins
Mrs. A.J. Jewitt
Ms. S. Johnson
Mr. T.S. Knibbs
Mr. K. Leatherby
Mr. S. Lett
Mr. I.R. Lloyd
Mr. A.H. McKnight
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Mrs. L. Richmond
Mr. K. Schofield
Ms. V. Seaman
Mrs. G. Sewell
Ms. C. V. Spruce
Mr. I. Sutton
Ms. D.M. Taylor
Mrs. P. Topping
Mr. R. Turner
Mr. R. Vincent
Mr. L. Walton
Mr. D. Williams

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

Audebert, Dr Fernando, Buenos Aires Univ, Argentina
Birou, Thierry, CEMES/CNRS Toulouse, France
Bishop, Dr Hugh, MIMIV Ltd, Abingdon
Brutti, Dr. Sergio, Univ. of Rome, Italy
Burgmann, Dr. Flame, RMIT Univ. Melbourne, Australia
Butler, Dr Paul, Crown Cork & Seal Co Inc, Wantage
Castro, Dr. R, Los Alamos Nat. Lab., USA
Cattaneo, Mr. Diego, Politecnico di Milano, Italy
Chang, Miss Lan-Yung, Univ Cambridge, UK
Chauke, HR, Univ. of the North, South Africa
Chen, Professor Xiaohua, Hunan Univ Changsha, PRC
Choi, Dr. Si-Young, Korea Advd Nat. Inst. S&T, South Korea
Dong, Dr Hongbiao, Imperial College London
Doyle, Dr Tony, Doyle & Tratt Products Ltd, Horsham
Eyre, Prof Brian, (retired chair of CCLRC)
Fairchild, Mr John, Forensic Alliance, Culham Science Centre
Falster, Dr Robert, MEMC Electronic Materials, Italy
Finnis, Prof Mike, Queen's Univ Belfast
Flewitt, Prof PEJ
Gabrys, Dr Barbara, Oxford Univ Dept Continuing Education
Gillespie, B.A., Univ. of Virginia, USA
Gilmour, Dr. B., Dept. Archaeology
Gilmore, Mr J., student, Univ. of Queensland, Australia
Gotora, Dr Duce, Zimbabwe
Gruenbaum, Prof. E., Univ. Tel Aviv, Israel
Hashimoto, Dr A, Natl Inst Adv Science/Technol, Tsukuba
Imeson, Dr Doug, DSTL
Jefferson, Prof JH, Qinetiq
Khlobystov, Dr. Andrei, Univ. Nottingham, UK
Kiselev, Prof. N.A., Inst. Of Crystallography, RAS, Russia
Kolosov, Prof. V., Ural State Econ. Univ., Russia
Kugler, Prof Sandor, Budapest Univ Technol/Econ, Hungary
Lemoine, Stephane, University of Rouen, France
Marks, Prof. Laurence, Northwestern University, USA
Matijasevic, M., SCK-CEN, Belgium
Muhl, Dr. Thomas, Leibnitz Inst. for solid state, Dresden, Germany
Mukhopadhyay, Dr Sangamitra, Inter-Univs Indora, India
Myhra, Dr. S., Griffith Univ. School of Science, Queensland
Ogura, Tomo, Tokyo Institute of Technology, Japan
Park, Prof. Myung-Beom, Kroea 3rd Military Academy, Korea
Poullainm, Prof. Giles, University of Caens, France
Ramsack. Prof. Toni, University of Ljubliana, Slovenia
Schönberger, Dr Uwe, Max-Planck Inst, Stuttgart
Smith, Dr Peter, GCHQ
Swan, Mr Mark, Radcliffe Infirmary, Oxford
Tohmori, Mr Masashi, Univ. of Shiga Prefecture, Japan
Usher, Prof. A., Latrobe University, Australia
Valladares, Dr. A., Nat. Univ. of Mexico
Visart de Bocarmé, Dr Thierry, Free Univ Brussels, Belgium
Wu, Dr Houzheng, Coventry Univ
Yi, Prof Jianhong, Central South Univ, Hunan, China
Yianno, George, student, Cambridge University, UK
Yung, Man-Hong, University of Illanois, USA
Zhao, Dr Kunyu, Kunming Univ. of Sci&Tech., PRC
Zurob, Dr Hatem, Polytecnic de Grenoble, France

Alumni Association Committee

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Dr. G.R. Armstrong, Chief Materials Engineer, Goodrich Actuation Systems / Lucas Aerospace
Dr. E. Boswell, Procter and Gamble
Dr. M.H. Burden OBE, Technical Director, Dowty Aerospace Propellers
Mr. H. Dickinson, MD, Norton Aluminium Products Ltd.
Professor R.D. Doherty, Drexel University
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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
Mr. R. Strawson, Head of Physics, Abingdon School
Professor G.D.W. Smith, FRS, Department of Materials, University of Oxford

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Professor B.L. Eyre, CBE, FRS, FREng, formerly Chairman CCLRC
Dr S. Garwood, Director of Technology, Aerospace Dept., Rolls Royce plc
Mr. R. Malthouse, Group Secretary, Cookson Group
Dr. C.C. Morehouse, Director, Information Storage Technology Lab, Hewlett-Packard USA (Committee Chairman)
Dr. J. Patterson, Head of Fuel Cycle Technology, British Nuclear Fuels
Professor C.J. Peel, Director, Technology (Strategy), FST, QinetiQ Ltd
Prof. Y. Tsukahara, Toppan Printing Co., Japan

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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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British National Space Agency
Chinese Government
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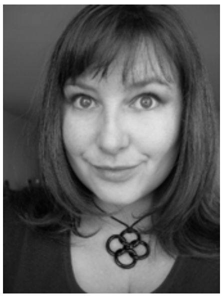
Wellcome Trust

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.



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.

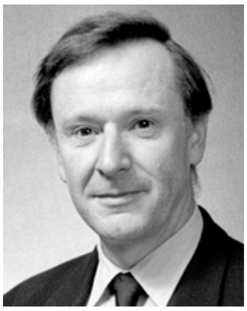
Dr. Roger Booker **Emeritus Reader in Electronic Materials**
Wolfson College **OCAMAC Senior Fellow**

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. David Bucknall — **Visiting Lecturer in Materials**

Structure and morphology of polymers. Effects of molecular architecture on polymer diffusion and structure. Influence of external fields in determining and controlling chain orientation and segregation behaviour. The structure and dynamics of polyrotaxanes. Nano-scale molecular devices derived from polyrotaxanes. Use of neutron reflection and ion beam depth profiling techniques for studying surfaces and interfaces. Non-conventional lithography using polymers. Microfluidics. Digital ink-jet technology.

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.

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 light weight 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.

- 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. Recent interests include modelling the brittle-ductile transition and plastic properties of intermetallics.

- 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

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. Amit Kohn **RAE/EPSRC Research Fellow**

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

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. Christiane Nörenberg **Royal Society Dorothy Hodgkin Fellow**
Wolfson College

Growth of quantum nitride nanostructures (InGaN, AlGaN) by molecular beam epitaxy (MBE) and in-situ surface characteristion by elevated-temperature scanning tunnelling microscopy (STM) and electron diffraction to investigate nucleation and elucidate growth modes. Atomic-scale studies on the growth of metals on GaN surfaces. Investigations of the electronic structure of endohedral fullerenes by STM for possible applications in QIP.

Dr. Peter Northover **Lecturer in Materials**
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.

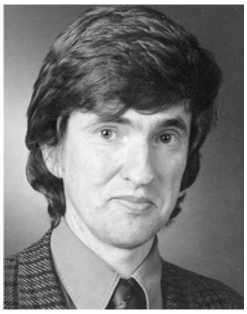
Dr. Keyna O'Reilly **Lecturer in Materials**
The Queen's College

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.

Dr. Steve Roberts **Reader in 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.

Dr. Jeremy Sloan **Royal Society University Research Fellow**
Wolfson College **(joint with Department of Chemistry)**

Synthesis and low dimensional crystal growth behaviour of low dimensional materials formed within single and multi-walled carbon nanotubes. Synthesis and characterisation of inorganic fullerene-like structures. Physical properties determination.

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

Semiconductor nanostructures and devices, particularly for use in quantum optoelectronics and quantum information processing. Design and characterisation of novel semiconductor nanocrystals for wide ranging applications such as sensors, fluorescent labels, photovoltaics, and telecommunications. Use of optical microcavities for controlled interaction between light and matter.

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

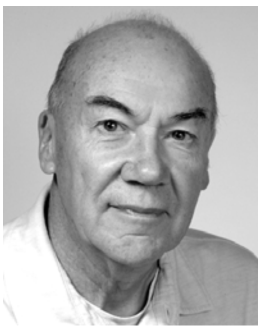
Processing of High Temperature Superconducting thin films on flat and curved substrates for a range of device applications. Recent work has focused on grain boundary properties and texture development in Tl-based HTS films. A growing area of interest is the development of superconducting meta-materials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

Dr. Ian Stone **Senior Research Fellow**

Processing-microstructure relationships in alloys and metal matrix composite systems. Evolution of microstructure during the spray forming process, grain growth in the semi-solid state, deformation behaviour of semi-solid alloys. Squeeze casting and rheocasting of wrought alloys. Manufacture and characterisation of amorphous, nanocrystalline and quasicrystalline aluminium alloys.

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.



Dr. Glyn Taylor **Senior Research Fellow**
Linacre College

Mechanical properties of metallic materials, especially the deformation of single crystals. Growth of single crystals for deformation studies, bcc metals and alloys containing oxide or nitride dispersions, intermetallic compounds including γ-TiAl and various B2 compounds. Relating yield stress and strength to the properties of dislocations. Measuring elastic constants.

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 (~10(measurements of stresses in metals and ceramics, and high spatial resolution surface studie superplastic flow.

- 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 degredation, 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 **Lecturer in Materials**
St Anne's College

Characterisation of the electrical and mechanical properties of defects in semiconductors. Development of novel structures and materials for field emitters to be used in field emitter displays. 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

I - MECHANICAL PROPERTIES OF STRONG SOLIDS, METALS AND ALLOYS

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.

A nanoindentation study of slip transmission at grain boundaries

D. Randman, 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 nano-indenter, AFM, SEM and electron back scatter diffraction to study conditions under which slip transmission occurs at boundaries of different character in an alpha Ti alloy. 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.

Development of corrosion resistant high strength ferritic steels

*Professor J.M. Titchmarsh, M. Briceno-Gomez, Dr. P. Brown**

High strength ferritic steels are prone to stress corrosion cracking. This project aims to improve cracking resistance by modifying the composition of Ni-Mo-containing ferritic steel by selected elemental additions. Alloys will be made by melt spinning and mechanical and corrosion properties optimised by systematic variation of heat treatment and microstructural characterisation. (*QinetiQ) (Funded by QinetiQ)

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. M. Tanaka, 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 – 450 K. 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.

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)

In situ SANS investigation of cavitation in superplastic alloys

*Dr. R.I. Todd, Dr. S. van Petegem**

The nucleation and growth of cavitation during superplastic deformation is being investigated using Small Angle Neutron Scattering at the SINQ neutron source in Switzerland. An in situ investigation of a model Sn-Pb-Cu alloy is being performed, and cavitation in Al 7475 will also be investigated (*Paul Scherrer Institute, Switzerland).

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.

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)

Properties of Super-elastic β Ti-Nb Alloys ('Gum Metal')

Dr. A.J. Wilkinson, Dr. R.I. Todd, D. Armstrong

A Japanese group have reported a β-Ti alloy 'Gum Metal' having very unusual mechanical properties (enormous elastic limit of ~2.5% strain, high tensile strength of 1-2GPa, low Young's modulus of 40-80 GPa). Amazingly they claim that plastic deformation of Gum Metal does not involve dislocation motion. The project will explore the processing, structure and properties of Gum Metal using powder processing, focused ion beam micromachining, nano-indentation and electron microscopy techniques.

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)

Deformation of single crystals of Nb-Zr-O alloys and Nb-Zr-N alloys

Dr. P. Manyum, Dr. G. Taylor*

Single crystals of niobium zirconium alloys are being oxidised at low pressures in an ultra-high vacuum furnace to produce a zirconia dispersion. The size of the precipitate is controlled by a subsequent anneal at ~1600C. Mechanical properties are being studied by differential tensile tests and the particle-matrix structure and dislocation-particle interactions observed by transmission electron microscopy. Similar experiments on Nb-N solid solutions are being carried out also at deformation temperatures well below ambient.

II – INTERMETALLICS

Mechanical properties of CoTi based alloy single crystals

L. Zhang, Dr. G. Taylor

CoTi crystals show a yield stress anomaly characteristic of certain intermetallic compounds. The peak-stress temperature and strength of the stoichiometric binary alloy are relatively low. The addition of isostructural CoHf is expected to increase these parameters significantly. Crystal growth is inhibited by the formation of Ti oxides and the deformation is characterised by glide of <100> dislocations.

Deformation of γ-TiAl single crystals with [001] orientation

S.J. Pak, Dr. G. Taylor

Single crystals of γ-TiAl have been grown with a [001] orientation from high purity alloys in the range 53.5-56 at%Al. They are being deformed deformed in compression and also in tension over a range of temperatures to study the yield stress anomaly and mechanical twinning. Selected slices are being analysed for dislocation content by TEM.

The growth and deformation of $TiAl_3$ single crystals

Dr. P. Manyum, Dr. G. Taylor*

Transition metal additions to $TiAl_3$ are being made to stabilise the cubic structure. Single crystals will be grown and used for deformation studies.(*Suranaree University of Technology, Thailand)

Crystal growth and mechanical properties of RuAl alloys

S.J. Pak, Dr. G. Taylor

The ruthenium aluminium system forms an intermetallic compound with the B2 structure at 50 % Al. RuAl has a high melting point and the vapour pressure of Al when the alloy is molten is sufficiently high to make the growth of single crystals difficult. A floating-zone crystal growth apparatus has been constructed for operation at above ambient pressure in an attempt to grow good quality crystals of RuAl and other B2 intermetallic compounds.

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B. Non-Metallic Materials

I - CERAMICS AND COMPOSITES

Perovskite-based ceramic nanocomposites

H. Wang, 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)

Environmental effects on surface damage in float glass

J. Minshull, Dr. P.D. Warren, Dr. S.G. Roberts*

Float is known to be more damaged on one side (the "tin side") by debris on rollers in the float line, but it is not clear where and how this damage occurs, nor how the strength of the glass depends on the damage. The project uses high-temperature indentation testing to investigate the mechanisms of surface damage accumulation in the float glass process, in particular the influence of surfactants. (*Pilkington plc)

High temperature strengthening of zirconia ceramics

M.P.S. Saran, Dr. R.I. Todd

Transformation toughening in zirconia is lost at high temperature owing to the reduction in driving force for the martensitic transformation which causes it. Cold pre-stressing is being explored as a method of retaining strength at high temperature. (In collaboration with Morgan Matroc)

Nanocomposite ceramics for technical applications

I. Shapiro, Dr. S.G. Roberts, Dr. R.I. Todd, Professor J.M. Titchmarsh

The project is aimed at understanding the behaviour of alumina - silicon carbide ceramic nanocomposites in applications where wear and abrasion resistance are important. There are two main aims - (a) to understand the mechanisms of their improved properties over normal alumina ceramics, especially their improved grain boundary strength; (b) to produce materials usable in real industrial applications. (Funded by EPSRC)

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)

Composites based on synthetic opal

*Dr. J.L. Hutchison, Professor L.M. Sorokin**

Novel composites have been prepared by filling the regular voids in synthetic opal by guest materials such as tellurium, InSb, GaAs, etc.. The opal is a cubic-close-packed lattice of SiO_2 spheres, and it has been found that the guest materials may be present as single-crystalline, 3-D networks, giving unusual properties. (*In collaboration with the Ioffe Physical-Technical Institute, St Petersburg, Russia, supported by the Royal Society)

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.

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

Stress measurement in alumina and other oxides using the shift of Cr^{3+} 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 Cr^{3+} cathodoluminescence given off by Cr-doped alumina in the electron beam of an SEM. (* Gatan Ltd.)

Carbon nanotube reinforced ceramics

T.T. Chu, Dr. J. Sloan, Professor M.L.H. Green, 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.

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.

II - BIOMEDICAL MATERIALS

Properties of biocomposites

Dr. J.T. Czernuszka, T. Williams

Composites based on natural systems are being made and their dynamic and static properties are being determined. New models of how this class of materials behave are being formulated. (Supported by the Rhodes Trust)

Tissue Engineering and three-dimensional scaffolds

Dr. J.T. Czernuszka, Dr. E. Sachlos, D.Wahl, Dr. C. Liu, J. MacBride

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.

Macro-assembled spheres of apatite

Q. Xu, Dr. J.T. Czernuszka

Lipid spheres are being coated with apatite which are 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)

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)

Nanolaminated composites

Dr. J.T. Czernuszka

Biochemicals are reacted with inorganic salts to form layered structures compromising alternating monomolecular sheets of biochemicals and ceramic monolayers. These materials possess novel ferro-electric, elastic and optical properties.

Design and fabrication of ceramic: biochemical: polymer composites

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

Additions of biochemicals, 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)

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 Elétrica e de Computação, Universidade Estadual de Campinas, Brazil)

Three Dimensional Scaffolds for Tissue Engineering

D. Wahl, Dr. E. Sachlos, 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. (*Begbroke Technology Centre; **Dept. Engineering Science, University of Oxford; ***Manchester Materials Science Centre) (Funded by EPSRC, DTI and the Wellcome Trust)

Tissue Engineering of Heart Valves

Dr. E. Sachlos, Dr. J.T. Czernuszka, Professor Sir Magdi Yacoub, Dr. P. Taylor*, Dr. A. Chester*, S. Dreger*, D. Gotora*

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 dsytematic 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)

Cleft palate repair

M. Swann, T. Goodacre**, Profesor J. Meakin*, Dr. D.G. Bucknall***, Dr. J.T. Czernuszka*

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)

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. (*Dunn School of Pathology, University of Oxford)

Nanoscale Mineralization of Response to Biomedical Composites of Resorbable Polymers and Apatitic Particulates.

T. Lim, Professor L. Hobbs , Dr. A. Garratt-Read*, Dr. H. Wang*, Dr. J.T. Czernuszka*

This project is in collaboration with Smith and Nephew Inc and it will investigate the morphology, kinetics and responses of implanting a certain type of resorbable material as bone screws into bone. (*MIT, Boston, Mass, USA)

III - POLYMERS

Electric Field Induced Orientation of Zwitterionic Telechelic Polymers

J. Xu, Dr. D.G. Bucknall, Dr. L.R. Hutchings, Professor R.W. Richards**

Zwitterionic telechelic polymers are ionomers with oppositely charged end-groups, which in solution can cluster into aggregates or behave as single chains depending on the polarity of the solution. We have been using electro-optic Kerr birefringence to understand the complex solution properties of these novel polymers. Due to the presence of the permanent dipoles on the chain ends orientation effects are highly sensitive to aggregation behaviour allowing different field alignment effects to occur. The segmental orientation of the chain therefore acts to produce an optical switch. (*IRC in Polymer Science and Technology, Durham University) (Funded by EPSRC)

Patternation of Polymer Thin Films

Dr. D.G. Bucknall, Professor G.A.D. Briggs, T. Okayasu

Thin polymer films can demonstrate interesting dewetting behaviour on non-wetting surfaces. By capping such unstable thin films by thick rigid layers this dewetting can be prevented. By selectively capping these inherently unstable thin films by semi-rigid capping layers it is possible to produce a surface topology with a random wave morphology. This project aims to understand this phenomena and ways to control the feature size and more particularly anisotropy of the resulting structures.

Network formation in epoxy/amine resins

D.L. Morgan, Dr. H.E. Assender

The formation of the network structure during the cure of a thermosetting resin depends on the relative reaction rates of the functional groups available, these are determined by the kinetics of the pure reaction chemistry and increasingly as the material gels the availability of reactive groups. FTIR spectroscopy and DSC analysis are used to study these reaction processes on a series of model compounds to determine the network structure that results.

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.)

Coating polymer films

*D. Howells, Dr. H.E. Assender, Dr. B.M. Henry, Dr. J. Robinson**

The project seeks to improve understanding and control the influence of a polyester substrate on subsequent coatings. The work would seek to identify factors that control the performance of a film as a substrate for subsequent coating, and to try various surface pretreatments to monitor their characteristics and effect. One major consideration will be the role of the topography of the substrate on subsequent coating performance. (*DuPont Teijin Films) (Funded by DuPont Teijin Films and EPSRC)

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.

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)

Nanopatterning with block copolymer thin films

T. Pickthorn, Professor R.A. Register, Dr. H.E. Assender*

Thin films of diblock copolymers make excellent contact masks for surface patterning, which we have 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 both: 1) the application of recently developed techniques for nanostructure alignment to the fabrication of inorganic nanostructures of interest in electronic devices, such as electronic circuitry and magnetic storage, and 2) elucidation of the mechanism and kinetics of the alignment process, and the factors controlling them. (*Princeton University, 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.

Oxidative degradation of polymers

L. Castro-Diaz, Dr. D. Vesely, Dr. H.E. Assender

The mechanism of oxidation is investigated from the point of view of formation and diffusion of free radicals. Dispersion, solubility and diffusion of anti-oxidants are correlated with Oxidation Induction Time test for different antioxidants. Evaporation and degradation of anti-oxidants, as well as oxidation rates of polyolefins in different halogen environments are investigated. The main aim is the explanation of the mechanism in which the oxidation results in loss of mechanical properties. (Funded by Linacre College and Regenesys)

Diffusion and solubility in polymers

G. Bernardo, Dr. D.Vesely, Dr. D.G. Bucknall

Accurate measurement of diffusion rates, solubilities and concentration profiles are used to establish thermodynamical parameters, which can explain the observed mechanism of diffusion process. Polymer solvents, as well as compatible polymers with upper and lower critical solubility temperatures are investigated. Two component phase diagrams are compared with three component phase diagrams, in which the third component is a solvent or a compatibilizer. The results are used to advance our understanding of the formation of microstructure in immiscible, miscible and compatibilized polymer systems.

Diffusion in composite materials

M. Zhu, Dr. D. Vesely, Dr. D.G. Bucknall

Diffusion of compounds through inhomogeneous polymeric materials is investigated from the point of view of diffusion rate and solubility. The size and distribution of the second phase is taken into account for the calculation of the diffusion path and for the permeability. Several diffusion mechanisms are considered and compared with the experimental results..

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.)

Device manufacture and characterisation of organic photovoltaic materials

Dr. K.R. Kirov, Dr. H. Smith, 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.)

Synthesis of novel organic materials for photovoltaic devices

B. Lochab, Dr. S. Amriou*, Dr. H.E. Assender, Dr. P.L. Burn**

For the development of novel organic photovoltaic materials, various organic materials will be synthesised for the construction of nanoscale architectures and improved device performance. (*Dyson Perrins Laboratory, Oxford University) (Supported by EPSRC and Toppan Printing Company Ltd.)

Deposition and characterisation of nano-porous conducting oxide films

Z. Xie, Dr. B.M. Henry, K. Kawata, Professor C.R.M. Grovenor

Conducting, transparent electrodes are a necessary component in polymer photovoltaic devices. The compatibility and interfacial electronic properties of oxide/polymer electrolyte composites are critical factors in determining the efficiency of these devices. This project is exploring sputtering, evaporation, sol-gel and anodising techniques to fabricate thin films with controlled microstructure. The optical and electrical properties of the films, and their compatibility with new functional polymers, is also being studied and correlated with the nanostructure of the films investigated by SEM, HRTEM and AFM. (Supported by the 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 a 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)

Organic photovoltaic materials

*R. Beal, Dr. H.E. Assender, Dr. J.M. Smith, Dr. P.L. Burn**

Organic photovoltaic materials exploiting novel polymers and other additives are being explored within test devices to determine photovoltaic behaviour and performance. (*Dyson Perrins Laboratory, Oxford University)

V - CARBON NANOMATERIALS

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)

Formation of Growth of Hybrid Carbon Nanomaterials

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

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 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. (*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)

Investigating the electronic structure of carbon nano-materials by STM

D.F. Leigh, Dr. C. Norenberg, Dr. S.M. Lee, Dr. A. Ardavan, Professor D.G. Pettifor, Professor G.A.D. Briggs

In order to fabricate a fullerene-based quantum information processing (QIP) device, we need to deposit 1-D and 2-D arrays of spin-active fullerenes with controlled spacing onto a suitable substrate. We are investigating small islands of various fullerenes, including C_{60}, C_{70}, Nd@C_{82}, Sc@$C_8$2 and Er3N@C_{82}, on a Ag/Si(111) substrate using variable-temperature Scanning Tunnelling Microscopy (STM), in conjunction with members of the Molecular Modelling Laboratory who are performing density functional theory (DFT) calculations for these molecules. At room temperature the fullerenes are mobile and diffuse across the surface to form compact islands. We observe their epitaxial relationship with the substrate, and their preference for adsorption at step edges, phase boundaries, and other inhomogeneous sites in the surface. At low temperatures (~77 K) the rotation of the molecules is frozen out and we can to resolve the molecular orbitals of these fullerenes directly. This gives a direct comparison to the calculated structures, and allows us to assess the interaction between the substrate and the fullerenes. We will conduct further analysis on the interaction between the fullerenes using Raman spectroscopy. Photoluminescence (PL) from optically active fullerenes will elucidate the possibility of optical addressing of a QIP device based on these species. Dual evaporation experiments will be used to investigate the interactions between different fullerene species. (Funded by EPSRC Foresight LINK award, DTI and Hitachi Europe).

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:C_{60} 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)

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)

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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. (*Inorganic Chemistry Laboratory) (Funded by EPSRC, Leverhulme Trust and The Royal Society)

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)

Bionanotechnology and carbon nanotubes: protein-functionalisation and biosensing

Dr. S. Contera, H. Hamnett*, N. Toledo*, K. Voïtchovsky *, 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)

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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 superconducting materials

Dr. H. Wu, Dr. S. Speller, S. Latif, R. Hitchman, A. Hardyment, Professor C.R.M. Grovenor*

Superconducting ceramic samples fabricated in thin film and 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. High resolution and analytical TEM and SEM, XRD texture analysis and orientation imaging microscopy techniques are being used to study the key microstructural features - especially the grain boundary structure and properties. (University of Coventry*)

Fabrication of thin films of Tl-2212

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

Sputtering and post annealing processes are being used to deposit thin films up to 3² in diameter of Tl-based superconducting ceramics, including films > 1 micron thick for novel THz devices. The mechanisms of growth and the composition and microstructure of the films are being investigated as a function of deposition parameters, and related to the superconducting and microwave properties. Vicinal and cylindrical substrates are also being used to achieve novel structures for specific device designs. The aim is produce optimised high Jc/low Rs materials for a wide range of practical applications. (University of Coventry*, Department of Engineering Science**) (Supported by EPSRC Grant GR/S42262 and the Royal Academy of Engineering)

Synthesis and microstructure of MgB_2 powders and wires

C. Dancer, R. Hitchman, A. Hardyment, Dr. H. Wu, Professor C.R.M. Grovenor, Dr. R.I. Todd, Dr. P. Kovac**, Dr. T. Prikhna****

MgB_2 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 MgB_2 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 . (*University of Coventry, **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. H. Wu, 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** and University of Coventry*)

Grain boundary properties in HTS thin films

Dr. S. Speller, C.J. Dark, Dr.A. Sundaresan, Dr. Y. Tanaka**, Dr P.Odier***, Professor C.R.M. Grovenor*

The properties and structure of grain boundaries in Tl-2212 and Tl-1223 thin films are being studied to correlate structure with critical current performance. New work on Hg-1212 grain boundaries is just starting with CNRS. Both artificial and natural grain boundaries are being grown on $LaAlO_3$ and MgO substrates, and doping of the boundaries to improve properties is also being attempted. The properties of these boundaries has been shown to fall very far from the accepted Jc/theta dependence found in TBCO films. (*Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore; **Nanoelectronics Research Institute (NeRI), AIST, Tsukuba, ***CNRS Grenoble, France) (Funded by EPSRC)

II - SEMICONDUCTOR MATERIALS

Room temperature light emission form 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. (*Gatan, UK; **MEMC, Italy) (With support from MEMC, Italy)

Impurities and dislocations in Si wafers

J. Murphy, 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 350-850°C 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, Italy) (Funded by EPSRC, MEMC)

New Detectors for Transmission Electron Microscopy

Professor A.I. Kirkland, Dr P.R. Wilshaw

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 framerate. 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)

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.)

Spectroscopy of Quantum Dot Quantum Wells

Dr. J.M. Smith, E. Tyrrell

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 tunable 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 of single ZnS / CdSe QDQWs grown by collaborators at the University of Manchester. We model data by calculating the electronic energy levels in the materials using a specialised 8-band Hamiltonian in spherical symmetry. (Preliminary funding for this project has been provided by the University's Research Development Fund)

Surface passivation of semiconductor nanocrystals

Dr. J.M. Smith, B. Sher

Semiconductor nanocrystals grown by wet chemical methods have enormous potential for use in quantum information applications. The unique quantum mechanical properties of electrons and holes in single nanocrystals can be exploited to build such devices as single photon sources, which could be used for quantum cryptography or even 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. This project will address ways to tackle the problem of surface passivation, including embedding the nanocrystals in thin films and studying novel "quantum dot quantum well" nanocrystals. The project will involve performing characterisation (primarily photoluminescence spectroscopy and time-resolved photoluminescence) on single nanocrystals, and analysing the effect of various novel growth methods on the drift and blinking phenomena. It will involve collaboration with a well established group at the University of Manchester Department of Chemistry, where the samples will be grown.

Electron field emission from dielectric and ferroelectric films

D. Jordan, Professor G. Poullain, Dr. P.R. Wilshaw*

Experiments are being performed with a view to understanding the mechanism by which electron field emission from flat surfaces can, in some circumstances, be improved by the deposition of a thin dielectric film. Preliminary experiments are using, as a model system, different thickness silicon dioxide films grown on silicon substrates. Work is also being undertaken on thin ferroelectric films. (*Lab CRISMAT, Caen University, France)

Optically induced degradation of Cz-silicon solar cells

P. Lewis, J. Murphy, 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 enahnced oxygen diffusion. (*MEMC, Italy)

Quantum wires and dots

Dr. J.L. Hutchison, X. Chen, 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.) (Funded by EPSRC and Oxonica Ltd.)

III - MAGNETIC MATERIALS

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 (μ-TAS). 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)

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)

Studies of patterned magnetic thin films

*T. Bromwich, Professor A.K. Petford-Long**

Thin magnetic films grown by sputter deposition and by molecular beam epitaxy are being patterned to form arrays of magnetic antidots. Further patterning of the films is being carried out using polymer self-assembly to form arrays of magnetic dots. The magnetic domain structure and magnetisation processes are being studied by Lorentz microscopy for correlation with microstructure. The films have applications as high density storage media (Funded by EPSRC)(*Argonne National Laboratory, USA)

MBE growth of epitaxial exchange-biased layers and 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 exchange-bias films, so that the exchange-biasing mechanism (vital to the operation of modern hard-disk read-heads) can be studied in the absence of features such as grain boundaries. The magnetisation reversal of the films is being characterised using Lorentz electron microscopy and their microstructure is being analysed using HREM and composition mapping. The project will also include the deposition and characterisation of epitaxial tunnel junction structures based on a variety of materials. (*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 Co_2MnSi 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)

Spin-tunnel junctions based on magnetic layered films

Professor A.K. Petford-Long, V. Jackson, Dr. A. Kohn, Dr. T.C. Anthony**, Dr. J.A. Brug***

Spin-tunnel junction devices are magnetic layered systems which exhibit giant magnetoresistance. The aim is to develop these systems for applications as magnetic field sensors and/or magnetoresistive memory elements. (*Argonne National Laboratory, USA. **Hewlett-Packard Labs.) (Funded by Hewlett-Packard Labs. and EPSRC)

Development of an MRAM device embedded on silicon

Dr. A. Kohn

The EMAC project which stands for ŒEmbedded Magnetic Components¹ 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).

IV – QUANTUM INFORMATION PROCESSING

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.

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)

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)

Endohedral Fullerenes for Quantum Information Processing

J.J.L. Morton, D.A. Britz, , M.A.G. Jones, 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 $N@C_{60}$). 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)

Logic Gates with Excitons and Spins in Quantum Dots

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. (In collaboration with Hewlett Packard Laboratories Bristol and Ben-Gurion University)

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)

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)

ESR Study of Carbon Nanostructures for Quantum Computing

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

Molecules of N@C_{60} 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)

Manufacture of HPLC Columns for Separation of N@C_{60}

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

N@C_{60} and C_{60} are difficult to separate, as they have virtually indistinguishable affinities for most materials. We have targeted their most apparent difference, mainly that N@C_{60} is more polarizable than C_{60}, 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)

Decoherence of Confined Excitonic States

Dr. B.W. Lovett, 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 and Ben-Gurion University)

Isolation and characterization of N@C_{60} derivatives

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

We have recently succeeded in adding useful functional groups to N@C_{60} and separating the material purity approaching 100%. These functional groups alter the spin properties of the molecule and may change important parameters for its use as a computational quantum bit. We find that certain functional groups do not have a substantial effect on these properties and thus still useful for quantum computation. The subtle changes imposed by the functional groups need to be further studied to determine the extent of their effect.(*Clarendon Laboratory, Department of Physics)

Towards Optical Readout of a Fullerene Quantum Computer

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

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)

Theory and modeling of spin-qubit interactions in nanotubes and fullerenes

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

This theory project is concerned with the interaction between spins of propagating and bound electrons in single-wall carbon nanotubes (SWNTs) and nanotube-fullerene systems. The aim is using first principles Hartree-Fock (HF) and density functional theory (DFT) to investigate the factors which govern these interactions which are relevant to the transfer of quantum information between spin-qubits. (*QinetiQ; **Rutherford Appleton Laboratory, CCLRC)

Dimers for quantum computing

J. Zhang, Dr. K. Porfyrakis, Dr. M. Sambrook, 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 ŒCluster-state¹) 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. 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)

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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.

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.

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)

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)

DC and shape casting of wrought Al alloys

*I. Davidson, Dr. K.A.Q. O'Reilly, Dr. I.C. Stone, Mr. M.R. Jarrett**

Control of intermetallic phase selection, via grain refinement procedures and minor element additions, is being investigated in D.C cast, squeeze cast and semi-solid processed conventionally wrought Al alloys.(*Alcoa) (Funded by Faraday Partnership and Alcoa)

Melt conditioning of Al alloys

M. Lovis, Dr. K.A.Q. O'Reilly, Dr. I.C. Stone, P.G. Enright**

This project is developing novel thermal and chemical melt conditioning procedures for the control of microstructures during casting, providing evaluation and measurement technologies for the same. (* N-Tec Limited) (Funded N-Tec Limited)

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)

Understanding the properties of semi-solid alloys during rheocasting

M.F.B. Holden, Dr. I.C. Stone, Dr. K.A.Q. O'Reilly

This project aims to deepen the understanding of the mechanical behaviour of semi-solid alloys through a range of solid fraction from that associated with rheocasting during die filling to that associated with the final stages of solidification when the solidifying alloy may be susceptible to hot tearing. Semi-solid alloy slurries are being produced. The microstructures are being characterised. The properties are being measured in compression and in tension using thermomechanical analysis, and correlated with the microstructure/ processing conditions.

The role of "metal health" on intermetallic phase selection and hot tearing

S.R. Holmes, Dr. I.C. Stone, Dr. K.A.Q. O'Reilly

This project is investigating whether the presence of extensive oxide inclusions in molten aluminium has an influence on the selection of Al-Fe-Si intermetallic phases that form during the late stages of solidification. Alloys are being prepared with various levels of 'health' (natural oxide content), and with deliberate additions of known oxide particles. The level of oxide content is being assessed and the role of these oxides on fluidity and hot tearing is being investigated using the 'metal health' suite of equipment. The type of intermetallics formed is being characterised. The mechanical properties of the alloys with a low volume fraction of liquid is being measured under conditions similar to those experienced during hot tearing.

Manufacture and characterisation of nano-quasicrystalline aluminium alloys

M. Galano, Dr. F. Audebert, Dr. I.C. Stone, Professor B. Cantor**, Professor G.D.W. Smith*

Al-based nanocomposite materials containing high volume fractions of quasicrystalline dispersoids are being produced by rapid solidification techniques. Particular emphasis is being placed on the microstructure stability and the mechanical properties leading to the manufacturing of the alloy in bulk shape.(*University of Buenos Aires; **University of York) (With support from Niobium Products Company GmbH)

Reliable compact capacitors for aerospace applications

*C. Hinchliffe, Dr. T. Starke, Dr. C. Johnston, Professor P.S. Grant, Professor P. Dobson**

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 Rolls-Royce plc and EPSRC) (*Academic Director of the Oxford University Begbroke Science Park,)

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).

Optimisation of spray forming of advanced high quality components of Ni super alloys for aeronautic applications

Dr. J. Mi, Dr. I.C. Stone, Professor P.S. Grant

The mechanism of refined, equiaxed grain evolution in spray forming, and the role of insoluble nitride, carbides and microporosity, are being investigated by a combination of manufacture of Ni preforms by spray forming under different processing conditions and microstructural characterisation by EPMA and phase extraction/XRD. The development of Ni superalloys which exploit the unusual solidification conditions in spray forming is also being explored in order to enhance high temperature strength and creep properties (Funded by EU Framework V and in collaboration with Bremen University, ITP, Turbomeca, BEG, MTU, BSTG, ALD, Inasmet)

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 spraycasting; 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).

Modelling, microstructure and properties of nickel superalloys processed by centrifugal spray deposition

*Dr. Z. Shi, Professor P.S. Grant, Dr. M. Ward**

The main scientific objective is to underpin the commercial and technological development of the Centrifugal Spray Deposition (CSD) process through improved scientific understanding. This will be achieved through the application of state of the art diagnostic techniques, systematic experimentation and the development of process models which better define the relationships between atomisation and deposition parameters, preform shape, microstructure and properties. Technical objectives are the spray forming of high performance Ni alloys (including IN718, Waspalloy and the Rolls Royce alloy RS5); the identification of deposition strategies consistent with the production of axi-symmetric components with extended axial length; and the production of medium-large diameter ring-shaped preforms with internal and external shape. The programme aims to provide, through innovative developments in materials processing, modelling and optimisation, an alternative high yield, cost-effective manufacturing route for the production of seamless ring and casing components for use in aeroengine, industrial and marine gas turbines (In collaboration with *Birmingham University and funded by EPSRC, DSTL, Qinetiq, Doncasters Ltd, Alstom, Bodycote HIP Ltd, Rolls-Royce plc).

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 Scholarship)

Nodal optimisation in truss structures

Ms S. Panteny, Professor P.S. Grant

Multi-material high stiffness, low weight 3D truss structures made from node and strut assemblies promise great benefits in structural engineering. Truss structures can be used as the building blocks for lower weight wing structures, enabling longer wings to be manufactured, while their excellent vibration resistance, high damage tolerance, and incorporation of stealthy materials makes them ideal for unmanned air vehicles (UAVs). Currently, truss structures have achieved only limited applications as the underpinning joining technology has yet to be developed and therefore potential weight savings and manufacturing costs have failed to meet expectations. This project is investigating innovations required to enable the wider implementation of truss structures in civil applications by: - the manufacture of lightweight demonstrators defined by end-users; - the investigation of enabling joining technologies; - the development of design and simulation software for complex 3D truss geometries; - the investigation of new node materials and their assemblies into truss structures; and - the development of joining technologies for repair. The project involves two universities, a research and technology organisation and five industrial partners. (Funded by Advanced Composites Group, Airbus UK, Carr Reinforcements, Crompton Technology, MIRA, Ellis Developments, Oxford Brookes University, DTI.)

Development of new applications for freeze cast near net shapes

J. Taylor, 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.

Thermal and electrical effects in composite films.

C. Wilkinson, Professor P.S. Grant

Non-conductive polymer films containing nano-sized and micron-sized conductive or other fillers are being made by a new spray deposition technique. Coating thicknesses in the range 10-50 microns are being produced and dielectric properties are being investigated as a function of fraction of particle, particle type and at elevated temperature. Critical to the production of high quality films is the formulation of appropriate colloidal suspensions suitable for spray processing and particular routes are being developed for each of the particle types of interest. The dynamics of the spray process are being investigated by high speed digitial video photography, the insights from which are being used to help explain as deposited film microstructure and other characteristics.

Advanced materials for plasma facing components (PFC) 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)

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 125 ^{o}C.

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 >100^{o}C 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)

Electronics Reliability

Dr. C. Johnston and Professor P.S. Grant

Reliability of electronic components, especially passives, packaging and interconnects for applications in extreme environments.

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E. Surfaces, Interfaces and Phase Transformations

I – OXIDATION AND CORROSION

Pitting of Stainless Steels

J.M. Sykes

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

Ageing of organically coated metal surfaces

E. Whyte, Dr. J.M. Sykes, Dr. H.E. Assender, Professor G.A.D. Briggs

The project brings together experimental and predictive modelling approaches to the investigation of the degradation, or ageing, of polymer coatings applied to metal substrates. The project will combine data from electrochemical (EIS, scanning Kelvin Probe) experiments with physical and chemical information from acoustic microscopy, scanning probe techniques and surface chemical analysis in order to determine the key factors involved in the degradation of coating systems. (In collaboration with Corus)(Funded by EPSRC and Corus)

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)

II - SURFACE REACTIONS AND CATALYSIS

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)

Atomic scale studies of solute transport along grain boundaries

Professor A. Cerezo, Professor G.D.W. Smith

The objective of this work is to understand how solute diffusion along grain boundaries affects environmentally-induced degradation. (Funded by Ministry of Defence, in collaboration with Manchester University, Birmingham University and Johnson Matthey.)

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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)

Nanostructures on the $SrTiO_3$ (001) Surface

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

Atomically resolved scanning tunnelling microscopy of the $SrTiO_3$ (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)

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

*Dr. C. Norenberg, Dr. R.A. Oliver**

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. (*Dept. of Materials, Cambridge University)(Funded by The Royal Society)

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 $SrTiO_3$ 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.

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 structure of the islands are imaged with scanning tunnelling microscopy, and a variety of spectroscopic techniques are used to measure their electronic structure. (*DSTL)

STM of polar $SrTiO_3$ 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 $SrTiO_3$ (111) and $SrTiO_3$ (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.)

The surface structure of $SrTiO_3$ (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 SiO_2 transistor gate insulator in complementary metal oxide semiconductor (CMOS) devices. One of the major contenders for the material replacement is $SrTiO_3$. The purpose of the project is to investigate the surface reconstructions of $SrTiO_3$ 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.

Systematic control of the size and shape of epitaxial quantum nitride nanostructures

Dr. C. Norenberg, Dr. R.A. Oliver, Dr. V. Lebedev**, Dr. M.R. Castell, Professor G.A.D. Briggs*

The growth of self-assembled quantum nitride nanostructures (InGaN, AlGaN) by molecular beam epitaxy (MBE) is studied in-situ by elevated-temperature scanning tunnelling microscopy (STM) and electron diffraction to investigate nucleation and elucidate growth modes. The size and shape distributions of quantum dots are studied to develop a nanostructure diagram as a function of composition and growth parameters. (*Cambridge University, Department of Materials, **TU-Ilmenau, Germany)(Funded by The Royal Society)

Optical resonances of oxide nanostructures

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

Crystalline oxides such as $SrTiO_3$ 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 $SrTiO_3$ 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, Dr. C.-Y. You, 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, DTI and Oxford Nanoscience Ltd., and in collaboration with Hitachi Global Storage Technologies)

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 Oxford nanoScience, in collaboration with Hitachi Global Storage Technologies.)

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.)

3D Reconstruction of atom probe data

Dr. G. Chapman, Professor A. Cerezo*

Software for accurate 3-D reconstruction of data from the position-sensitive atom probe (PoSAP) is under continuous development. Algorithms include statistical functions for the detection of the early stages of clustering in alloys, and the use of Fourier transforms to permit detailed crystallographic reconstruction. (Funded by *Oxford Nanoscience Ltd.)

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

A. Gomberg, 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 Oxford nanoScience.)

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) eletron 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 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 parallel EELS (electron energy-loss spectroscopy) and an on-line TV system.

Analytical electron microscopy (AEM)

A Philips CM20, a modern 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).

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

Early 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 equiped 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.

Aberration-corrected electron microscopy

As part of the Departmental JIF grant, the Department recently 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 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.

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 either a gas environmental cell for in-situ studies under controlled atmosphere conditions, or with a low-field objective pole-piece for studies of magnetic materials. The unique gas environmental cell facility is capable of better than 0.3nm resolution whilst the specimen is surrounded by gas and held at elevated temperature. The instrument also includes x-ray microanalytical and electron energy loss spectroscopic (PEELS) facilities, together with an on-line TV imaging and recording system. With the low-field objective pole-piece inserted 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.

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 to be 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 will develop new collaborations in the chemical analysis of biological materials with colleagues in Oxford and elsewhere - the first of these will be on the study of metal species in hyperaccumulator plants, and in the mapping of radiopharmeceuticals in human tissue samples.

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,

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 a the 1 Å level. The instrument is being used for atomic-scale investigations of a range of new materials. (Funded by the Joint Infrastructure Fund)

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.

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)

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.

Polyhedral and cylindrical metal chalcogenides

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

Closed polyhedral structures of the layered materials WS_2, MoS_2 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. (*Weizmann Institute, Israel)

Development of FIB machining technologies

*Dr. Y. Huang, Professor J.M. Titchmarsh, Professor D.J.H. Cockayne, Professor A.K. Petford-Long**

Development and application of focussed ion beam machining technology for the preparation of specimens of analytical microscopy.(Funded by EPSRC platform grant)(*Argonne National Laboratory, USA)

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)

Structure of amorphous materials

Professor D.J.H. Cockayne, Q. Yao

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.

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)

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 1Å. 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 a 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)

3-D microstructural analysis using a FIB system

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

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)

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. (*Institute of Crystallography, Russian Academy of Sciences)

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***, S-J Shih*

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 EU and NSF between participants at *Max Plank Institute, Stuttgart, **University of Karlsruhe, ***CEA, Saclay, +MIT, ++University of Pennsylvania, +++Rutgers University, ÝUniversity of Missouri-Kansas; and ÝÝLawrence Berkeley Lab, San Francisco.

Electron Energy Loss studies of nanostructures

Professor D.J.H. Cockayne, Dr. D. Nguyen Manh, R. Nicholls*

The electron energy loss fine structure of fullerenes and other nanostructures is being investigated both theoretically and experimentally, using high resolution energy loss techniques and DOS calculations. (*UKAEA, Culham)

NanoSIMS analysis of metallic and electronic materials

S. Ahmed, Dr. M. Kilburn, 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] Grain boundary doping studies in high temperature superconductors (with University of Augsburg).

[2] Crack and grain boundary chemistry in structural steels (in collaboration with MOD and University of Manchester)

[3] Trace element chemistry in structural steels (in collaboration with Corus) Funding provided by EPSRC for DTA studentship for SA.

[4] Impurity and light element analysis in MgB_2 wires and powders (in collaboration with the Institute of Electrical Engineering, Slovak Academy of Sciences and the Institute for Superhard Materials, Ukraine).

NanoSIMS analysis of biomineralisation processes in marine coccoliths

Dr. R. Rickaby, Dr. M. Kilburn, 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). (Funded by EPSRC) (*Department of Earth Sciences)

NanoSIMS analysis of early life on earth

Professor M. Brasier, Dr. D. Wacey*, Dr. M. Kilburn, 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)

NanoSIMS analysis of Biological Materials

*K. Smart, G. Karney, Dr. M. Kilburn, Professor C.R.M. Grovenor, Dr. J.T. Czernuszka, Professor J. Dilworth**

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. Current projects include;

[1] the localisation of Rh complexes in a study of new imaging and therapeutic agents for hypoxic tissue.

[2] Trace element localisation in human hair and teeth (in collaboration with Proctor and Gamble).

(* Department of Chemistry)

Investigation of grain growth during fabriation 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)

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 has been put "on-line" in September 2005, and 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)

Interface Engineering of Multilayer Nanostructures

Professor M. Bilek, A/Prof. 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.

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.

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.

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)

TEM investigation of PRAM Materials and Devices

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

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 $Ge_2Sb_2Te_5$. 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 also collecting data from binaries. (*Samsung, Korea)

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)

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)

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

Dr. C. Lang, Professor Sir Peter Hirsch, Professor D.J.H. Cockayne

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. The accuracy of this approach is being investigated.

Fundamentals of Aberration Corrected Imaging in the TEM

Professor A.I. Kirkland

The department has installed the world¹s 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.

The structure and evolution of copper-rich precipitates in ferritic steels and their role in hardening

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

Hardening due to formation of copper precipitates is a major problem for in-service performance of reactor-pressure-vessel steels. The project aims to answers the following questions:

1. How do precipitate nucleation and growth, structure and composition depend on irradiation and thermal conditions?

2. What are the mechanisms of copper transport?

3. What is the effect of bcc-9R transformation on the copper-precipitate binding energy and overall kinetics?

4. What is the hardening mechanism of the coherent bcc precipitates?

5. Do dislocations cut through bcc precipitates, leaving them essentially unchanged, or do they induce transformation to the 9R structure?

6. What is the hardening mechanism of the incoherent 9R precipitates?

7. How are the mechanisms influenced by incorporation of other alloying elements?

(In collaboration with University of Liverpool and University of Illanois)

(Funded by EPSRC, Rolls-Royce and INSS)

IV - RADIATION DAMAGE

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

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

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)

Quantum Electron Microscope Imaging of Nanoclusters under Weak-Beam Conditions

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

This project is focused on the development of a new approach to the interpretation of electron microscope images of nanoclusters. 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. Our work involves development of a computer code implementing the original Howie and Basinski equations, to allow image simulations under weak-beam diffraction 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 interaction of high-energy particles with metallic crystalline films. (*Imperial College, **Argonne Natioal Laboratory, ***EURATOM/UKAEA)

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 600ºC, 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 steels based on iron ~9% chromium, vanadium alloys and tungsten. This project uses advanced techniques in electron microscopy to characterise the development of radiation damage in these materials. (Funded and in collaboration with EURATOM/UKAEA, * Argonne National Laboratory)

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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.

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).

Dynamical Ising model simulations of phase separation

Dr. G. Sha, A. Morley, Professor A. Cerezo, 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). (*BNFL Nuclear Sciences and Technology Services) (Funded by Rolls Royce)

Fatigue Crack Initiation in Polycrystals

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)

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 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)

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)

Current-induced effects in molecules

*M. Todorovic, Professor A.P. Sutton**

Current-induced mechanical and heating effects in molecular systems are being modelled. (Imperial College, London)

Mapping of magnetisation distributions in thin layered films

Professor A.K. Petford-Long, Dr. A. Kohn*

We have developed a method for quantitative mapping of the magnetisation in thin magnetic specimens at a high spatial resolution. The method is being used to study the magnetisation distribution in thin films and layered systems. In addition we are applying and developing the Transport of Intensity Equation approach for reconstruction of quantitative magnetic maps. (Funded by Hewlett-Packard Labs.)(*Argonne National Laboratory, USA)

Modelling carbon nanostructures for quantum computing

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

Tight binding and ab initio density functional codes are being used to predict the atomic and electronic structure and transport properties of single-wall carbon nanotubes containing endohedral fullerenes, which are being investigated in-house for their quantum computing potential. (*RAL **QinetiQ). (Funded by EPSRC Foresight LINK Project, DTI and Hitachi Europe).

Experimental and modelling studies of excitonic and charge transport in the organic-inorganic composite solar device

*K. Kawata, Dr. V.M. Burlakov, Professor G.A.D. Briggs, Professor I. Samuel**

Transport properties of excitons and holes in the conducting polymer, and those of electrons in inorganic semiconductor are being studied using spectroscopic and (photo)electrical measurements. Spectroscopic studies provide information about the diffusion coefficient of excitons and the charge separation performance of the organic-inorganic interface. Experimentally determined transport coefficients will be used in modelling of the solar device performance as a function of its morphology. (Funded by the Toppan Printing Company.) (*University of St Andrews)

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.

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)

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).

Theory and Modelling of Nano-morphology

Dr. A.S. Barnard

A new shape-dependent model is in development, capable of describing the thermodynamics of arbitary nanocrystals (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 s function of a number of experimentally relevant parameters such as size, temperature and surface chemistry, to compare the phase stability of polymorphs and to compare the relative stability of non-equilibrium shapes under desired conditions. (Supported by The Glasstone Trust)

Location and Coordination of Dopants in Nanocrystalline Diamond

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

Density Functional tight binding (DFTB) methods are being used to identify energetically preferred substitutional sites for the inclusion of experimentally relevant dopants 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 types of 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 dopants 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. (*Materials Science Division, Argonne National Laboratory) (Supported by The Glasstone Trust)

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)

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 phase change materials

Professor D.G. Pettifor, Dr. V. Burlakov, Dr. K. Kohary, Dr. J.A. Brug, Dr. T.C. Anthony*, Dr. C. Moorhouse**

The electron transport of phase change materials is being modelled by a Monte Carlo model of film growth and a Tight Binding model of conduction. There is close collaboration with the experimental Atomic Resolution Storage group at HP Laboratory. (*HP Laboratories, Palo Alto) (Funded by HP Laboratories).

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).

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)

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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 $6x10^3$ 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)

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).

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)

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)

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.

Iron Age silver in East Anglia

M. Dennis, Dr J.P. Northover*

Silver was virtually unknown in Britain before the late Iron Age and so its appearance in the 2nd/1st centuries BC is a decided novelty. For the first time this project looks at both coins and objects of silverware to discover how this ³new² material was understood and used and how it was deposited in the archaeological record. Both archaeological and metallurgical analyses are included. (*Institute of Archaeology, Oxford University)

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)

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)

Metalwork of the Bronze Age-Iron Age transition in Britain

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

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

R. McGhee, 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 ‘family trees’ 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)

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:

- Lightweight materials
- Reduced emissions
- End of vehicle life technologies
- The powered or blended wing
- The environmentally friendly aeroengine
- 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 (OMCS)

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.

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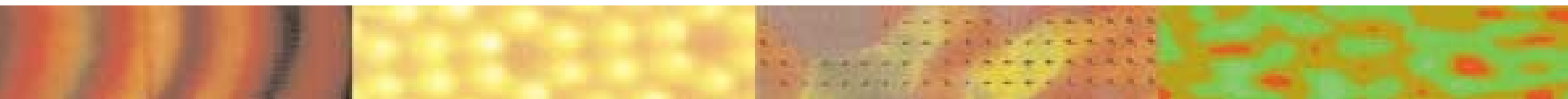

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