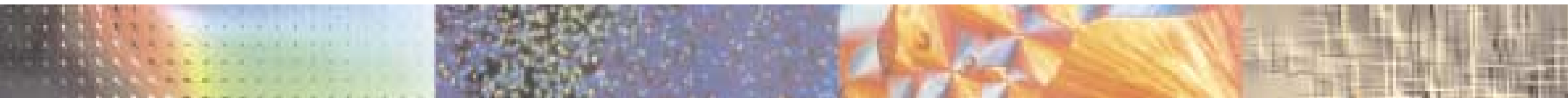
OxfordMaterials

Research in Progress
2003 - 2004

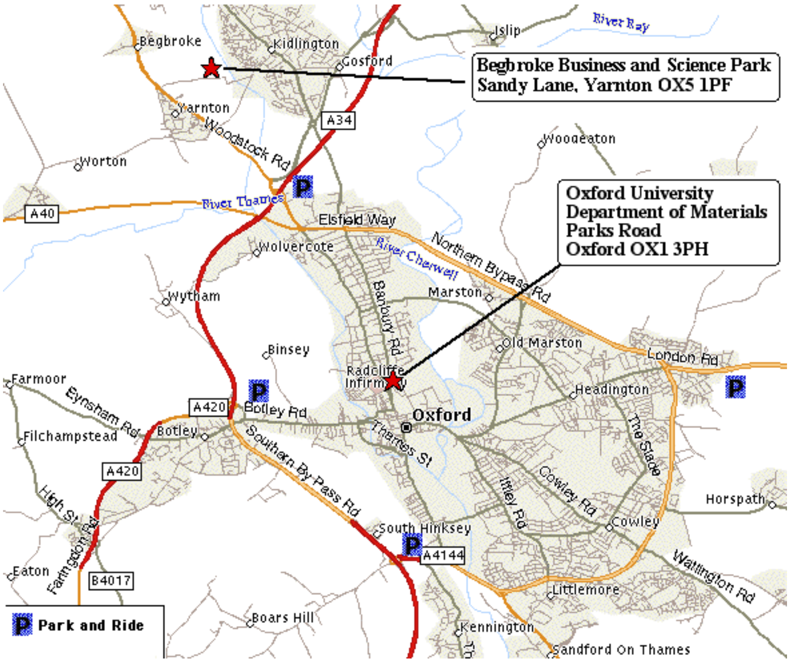


Department of Materials

Table of Contents

Department of Materials

University of Oxford



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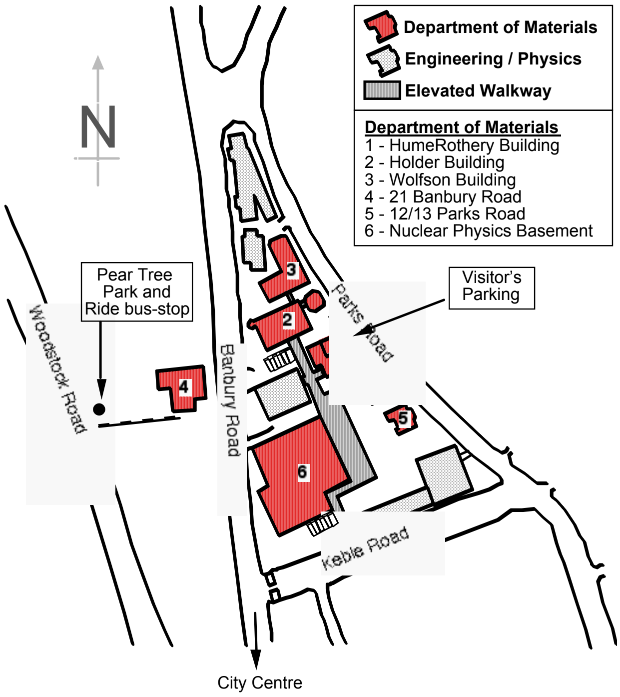
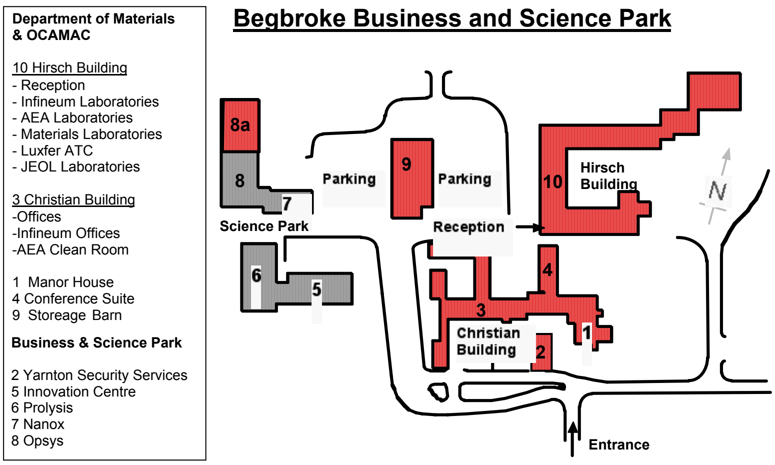
Keble Road Triangle



Begbroke Business and Science Park



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Foreword from the Head of Department

Welcome to 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.

Major achievements over the last five years include:

1. Three new Professorships in nanomaterials (Andrew Briggs), electron microscopy (David Cockayne) and structural integrity (John Titchmarsh);
2. Five elections to Fellowships of the Royal Society (David Cockayne, John Pethica, Brian Eyre, John Hunt and Adrian Sutton) and two elections to the Royal Academy of Engineering (Richard Brook and Brian Cantor);
3. Awards and honours to members of the Department, including 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 Beilby Medal and Prize (Alfred Cerezo), the Pfeil Award (Richard Todd), Metrology for World Class Manufacturing Awards (Andrew Briggs, Oleg Kolosov, John Hunt), and election to the US National Academy of Engineering and award of the Heyn-Denkmunze prize of the German Materials Society (Sir Peter Hirsch). Brian Cantor was appointed Vice-Chancellor of the University of York, Richard Brook received a knighthood, and was appointed Director of the Leverhulme Trust, 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).
4. Four promotions to personal professorships (Adrian Sutton, Amanda Petford-Long, Alfred Cerezo and Andrew Briggs) and six promotions to readerships (Patrick Grant, Chris Grovenor, 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 a Faraday Partnership in aerospace and automotive materials; and
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 was founded by Professor Hume-Rothery in 1956. At present, it consists of 24 academics, 16 senior researchers, 51 postdoctoral researchers, 38 technicians and administrative staff, 33 academic visitors, 92 research students and 101 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.

This booklet describes the full range of our current research programmes within the Department. 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. We are always pleased to discuss our research projects in more detail. We actively seek applications from new undergraduates, research students and research fellows, and we are keen to investigate further opportunities for collaboration and scientific exchanges. Please do not hesitate to contact us by letter, phone, fax or e-mail.

Professor G.D.W. Smith FRS
October 2003

Members of Department

Professors

Professor G.D.W. Smith, FRS	*Head of Department*
Professor D.G. Pettifor, FRS	*Isaac Wolfson Professor of Metallurgy* *Director of the Materials Modelling Laboratory*
Professor D.J.H. Cockayne, FRS	*Professor in Physical Examination of Materials*
Professor J.M. Titchmarsh	*The Royal Academy of Engineering/ AEAT / INSS* *Research Professor in Microanalysis and Structural Integrity*
Professor G.A.D. Briggs	*Professor of Nanomaterials* *Quantum Information Processing Interdisciplinary Research Collaboration*
Professor A. Cerezo	*Professor of Materials* *Director of Graduate Studies*
Professor A.K. Petford-Long	*Professor of Materials*
Professor A.P. Sutton, FRS	*Professor of Materials Science*
Professor Sir Richard Brook, OBE FREng	*Professor of Materials*
Professor J.B. Pethica, FRS	*Visiting Professor*
Professor C.R. Whitehouse	*Visiting Professor*
Professor J.V. Wood FREng	*Visiting Professor*
Professor Sir Peter Hirsch, FRS	*Emeritus Professor*
Professor J.D. Hunt, FRS	*Emeritus Professor*
Professor M.J. Whelan, FRS	*Emeritus Professor*

Readers

Dr. C.R.M. Grovenor	*Deputy Head of Department*
Dr. P.S. Grant	*Director of Oxford Centre for Advanced Materials and Composites* *Director of Faraday Partnership in Aerospace and Automotive Materials*
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. D.G. Bucknall	*Lecturer in Materials*
Dr. J.T. Czernuszka	*Lecturer in Materials*
Dr. P.J. Northover	*Lecturer in Materials*
Dr. K.A.Q. O'Reilly	*Lecturer in Materials*
Dr. R.I. Todd	*Lecturer in Materials*
Dr. P.R. Wilshaw	*Lecturer in Materials*

Administration

Dr. R.M. Plummer	*Administrator*
Ms. R.A. Meyrick	*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.I. Kirkland	Leverhulme Senior Research Lecturer
Prof. A. Balazs	OCAMAC Senior Fellow (Pittsburgh)	Dr. J.W. Martin	OCAMAC Senior Fellow
Dr. S.C. Benjamin	Royal Society Research Fellow	Dr. Duc Nguyen-Manh	OCAMAC Industrial Fellow (UKAEA)
Dr. R. Bhatti	Senior Visiting Fellow (QinetiQ)	Dr. C. Nörenberg	RS Dorothy Hodgkin Fellow
Dr. G.R. Booker	OCAMAC Senior Fellow	Dr. J. Sloan	Royal Society Research Fellow
Dr. M.R. Castell	Royal Society Research Fellow	Dr. I.C. Stone	Senior Research Fellow
Dr. S.L. Dudarev	OCAMAC Industrial Fellow (UKAEA)	Dr. G. Taylor	Senior Research Fellow
Dr. R. Falster	OCAMAC Industrial Fellow (MEMC)	Dr. D. Vesely	OCAMAC Senior Fellow
Dr. N. Grobert	RS Dorothy Hodgkin Fellow	Dr. P.D. Warren	OCAMAC Industrial Fellow (Pilkington)
Dr. B. Gilmore	Senior Visiting Fellow	Dr. A.J. Wilkinson	Royal Society Research Fellow
Dr. D. Imeson	Senior Visiting Fellow (DSTL)		

Research Fellows

Dr. R.J. Baxter	Dr. B.M. Henry	Dr. J. Leopoldes	Ms S. Panteny
Dr. V. Burlakov	Dr. C.J.D. Hetherington	Dr. B. Lovett	Dr. K. Porfyrakis
Dr. M J Carey	Dr. S.C. Hogg	Mr. M. Lovis	Dr. B. Reddy
Dr. A.M. Cock	Dr. Y. Huang	Dr. S. Lozano-Perez	Mr. C.J. Salter
Dr. A. Crossley	Dr. T.S. Hudson	Dr. J. Lynch	Dr. G. Sha
Mr. F. Cullen	Dr. C. Johnston	Dr. C.D. Marsh	Dr. Z. Shi
Dr. M. Döblinger	Dr. M. Kilburn	Dr. D.R. Mason	Dr. F. Silly
Mr. R.C. Doole	Dr. K.R. Kirov	Dr. R.R. Meyer	Dr. V. Suvorov
Dr. R. Drautz	Dr. A.N. Khlobystov	Dr. J. Mi	Dr. P.J. Warren
Dr. C. Dwyer	Dr. K. Kohary	Dr. J.H.G. Owen	Dr. S.J. Wilkins
Dr. A. Dupuis	Dr. A. Kohn	Dr. I.G. Palmer	Mr. G.B. Winkelman
Mr. T.J. Godfrey	Dr. S.M. Lee	Dr. D. Pankhurst	Dr. H-L. Zhang

D.Phil and MSc. Research Students

Abraham, M.H. (self-supporting)
Ahmed, S. (CASE: Corus)
Allsop, N. (EPSRC / St. Annes Scholarship)
Austwick, M.R. (EPSRC)
Bagot, P. (EPSRC)
Barkhouse, A (Rhodes Scholarship)
Barnes, J-P. (EPSRC)
Bernardo, G. (self-supporting)
Briceno-Gomez, M. (Qinetiq)
Britz, D. (EPSRC Foresight Link
Bromwich, T. (EPSRC DTA)
Brown, G. (CASE: Colebrand Ltd.)
Campbell, P.J.D. (CASE: BNFL)
Carter, R. (EPSRC)
Castro Diaz, L. (Regenesys / Linacre)
Chadd, G. (Crown Cork & Seal)
Chen, X. (self-supporting)
Choi, Y-S. (EPSRC)
Colley, L. (EPSRC)
Dark, C.J. (EPSRC DTA)
Davidson, I. (CASE: Alcoa Extrusions)
Davin, L. (EPSRC)

Deak, D. (EPSRC)
DeMorais, A. (Nordiko Ltd)
Di Maio, D. (Hardide)
Doherty, M.J. (EPSRC)
Eggeman, A. (EPSRC DTA + CASE: Johnson Matthey)
Galano, M. (EU/Korea/Clarendon/ORS)
Giannattasio, A. (MEMC Ltd.)
Gilberti, L (EPSRC)
Gomez-Morilla, I. (BNSC)
Gotora, D. (Rhodes)
Grennan-Heaven, N. (CASE: Oxford Nanoscience)
Gunlycke, D. (EPSRC Foresight Link)
Hinchliffe, C. (CASE: Rolls-Royce)
Howells, D. (CASE: Dupont)
Hudson, T. (AEA / Linacre)
Ito, F.
Jones, M. (EPSRC)
Joseph, T. (CASE: UKAEA)
Kawata, K. (Toppan Printing Co.)
Kirk, D. (EPSRC)
Kim, H.S. (self-supporting)
Kim, K-B. (self-supporting)
King, O. (EPSRC)
Korsah, M. (EPSRC)
Kurum, E. (EPSRC)
Lambourne, A. (Department)
Lang, C. (EPSRC)
Langham, C. (Motorola)
Leigh, D. (EPSRC Foresight Link)
Manson-Whitton, C.D.J. (Royal Commission for the Exhibition of 1851 Scholarship / Luxfer Ltd.)
Martin, C. (EPSRC)
Mathieson, D. (OPSYS)
Morgan, D.L. (EPSRC)
Morley, G. (EPSRC Foresight Link)
Morton, J. (EPSRC DTA / NEDO
Murphey, J. (EPSRC)
Nazir, A. (EPSRC)
Newell, D. (CASE: Oxford Applied Research)
Nicholls, R. (EPSRC DTA, St Catherine's Scholarship)
Nzula, M. (visiting student, Sainsbury Scholarship)
Okayasu, T. (Oji Paper Co.)
Oliver, R.A. (EPSRC)
Owen, N.W. (EPSRC)
Pak, S.J. (Self-supporting)
Park, S-B. (self-supporting)
Pinitsoontorn, S. (Thai Gov.)
Ramanujan, C.S.
Russell-Stevens, M.J. (EPSRC)
Sachlos, E. (St. Peter's College)
Saran, M. (Perdana Exchange Programme)
Saunders, S. (CASE: National Physical Laboratory)
Scipioni, R. (Self / EPSRC Foresight Link)
Shapiro, I. (EPSRC DTA)
Shinotsuka, K. (self-supporting)
Smart, K. (EPSRC)
Speller, S (EPSRC)
Srimanosaowapak, S. (Thai Gov.)
Stowe, D.J. (EPSRC)
Taylor, R.N. (CASE: Nanox)
Thomas, G. (CASE: UKAEA)
Todorovic, M. (Scatchered Scholarship)
Vaumousse, D. (CASE: Alcan International Ltd.)
Vlandas, A. (EPSRC, St Cross College)
Wahl, D. (EPSRC)
Wain, N. (EPSRC)
Waller, J. (EPSRC)
Walpole, A. (EPSRC DTA)
Wang, H. (Clarendon/ORS)
Waring, M. (EPSRC DTA)
Whiteley, R.M. (EPSRC)
Whyte, E. (CASE:Corus)
Wilkinson, S. (EPSRC / Guy Newton Wolfson Scholar)
Womersley, H. (EPSRC)
Xie, Z. (Clarendon /ORS)
Xu, J. (self-supporting)
Zhang, J. (Clarendon, ORS, Queens College)
Zhang, L. (ORS)
Zhou, Dr Z. (UKAEA)
Zhu, M. (K.C.Wong / ORS)

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

Part II Students (4th Year Undergraduates)

Materials Science

Beesley, E
Boden, S
Bruen, M
Copley, C
Creighton, C
Edwards, C
Fraser, K
Green, A
Haigh, S
Hodge G
Kirkby, E
Lee, SH
Morley, A
Powell, A

Materials, Economics and Management

Goodall, JBM
Hutchins, JD
Lindsten, J
Osborne, RD

Engineering and Science of Materials

Chapman, HA
Roberts, RH
Sykulska, HM
Woolmer, TJ
Hill, A

Secretarial and Technical Support

Mr. P. Abbott
Mr. S. Aldworth
(Mr. A.B. Bailey)
(Mr. S. Boyce)
Mr. M. Brechin
Mr. M.J. Carr
Mrs G. Chapman
Mr. R.E. Clemons
Mr. G. Cook
Mr. T. Cook
Mr. R.M. Cripps
Mr. R. East
Mrs. K. Fewings
(Mr P. Flaxman)
Mr. B.J. Fellows
Mrs. H. Fishman
Mrs. P. Gordon
Mrs. K. Hartwell
Mr. M. Hedges
Mrs. A.J. Jewitt
Mr. S. Kidsley
Mr. T.S. Knibbs
Mr. K. Leatherby
Mr. S. Lett
Mr. I.R. Lloyd
Mr. A.H. McKnight
Mr. M. Purches
Ms. K. Rana
Mrs. L. Richmond
Mr. K. Schofield
Ms. K. Sims
Ms. D.M. Taylor
Mrs. P. Topping
Mr. R. Turner
Mr. R. Vincent
Mr. L. Walton

Visiting Academics (2002-2003)

Dr F E Audebert, University of Buenos Aires, Argentina
Prof A C Balazs, University of Pittsburgh, USA
Dr R Bhatti, QinetiQ, UK
Ms C Bishop (graduate student), MIT, USA
Dr H L Brown, University of Minnesota, USA
Dr P Butler, Crown Cork & Seal Co Inc, UK
Miss L-Y Chang, University of Cambridge
Mr R H Chauke (graduate student), University of the North, South Africa
Dr D Crespo, Catalan Polytechnic University, Spain
Dr H Dong, University of Oxford
Dr A J Doyle, Doyle & Tratt Products Ltd, UK
Dr S.L. Dudarev, UKAEA, UK
Prof B L Eyre, Central Laboratory of the Research Councils
Dr R Fairchild, Forensic Alliance, Culham Science Centre
Dr R Falster, MEMC Electronic Materials, Italy
Dr B J Gabrys, Dept of Continuing Education, Oxford
Mrs S Gillis (graduate student), University of Minnesota
Dr B J J Gilmour, University of Oxford
Prof E Gruenbaum, University of Tel-Aviv, Israel
Miss R E Harper, Accentus, UK
Dr D Imeson, DSTL, Farnborough
Dr B J Inkson, University of Sheffield, UK
Dr S Jiansirisomboon, Chiang Mai University, Thailand
Prof N A Kiselev, Russian Academy of Sciences
Dr P Kovac, Institute of Electrical Engineering, Slovak Academy of Sciences
Dr D L Larson, Seagate Technology, USA
Miss T K Li, Chinese University of Hong Kong
Prof B-G Liu, Chinese Academy of Sciences, P R China
Ms B Maldonaldo, Penn State University, USA
Dr M Martín-Fernández, University of Oxford
Dr R Meyer, University of Cambridge
Dr K Miki, NIMS, Tsukuba, Japan
Dr S Mukhopadhyay, InterUniversities Consortium for DAE Facilities, India
Dr S Myhra, Griffith University, Australia
Dr Peter Northover, University of Oxford
Dr J C Oh, Centre for Advanced Aerospace Materials, Kyungbuk, Korea
Mr M Phasha, (graduate student), University of the North, South Africa
Dr Prof C J Peel, QinetiQ, UK
Prof L-M Peng, Chinese Academy of Sciences, P R China
Prof J B Pethica Trinity College Dublin, Republic of Ireland
Dr A Schneider, Max Planck Institute for Iron Research, Düsseldorf, Germany
Dr U Schönberger, Max-Planck Institute for Solid State Research, Germany
Dr S Senkader, University of Exeter, UK
Dr P Smith, GCHQ, UK
Dr C Sofield, Oxford [no affiliation]
Prof J Sun, Shanghai Jiao-tong University, China
Mr M C Swan, Radcliffe Infirmary
Miss K Titmuss, University of Cambridge
Dr T V Visart de Bocarmé, Free University of Brussels
Prof E Wang, Chinese Academy of Sciences, P R China
Dr. P.D. Warrren, Pilkington, UK
Prof C Whitehouse, Central Laboratory of the Research Councils
Prof J V Wood, Central Laboratory of the Research Councils
Dr H Wu, University of Coventry
Prof H Yang, Wuhan University of Technology, P R China
Prof F Zhang,
Dr Z Zhen, Beijing University of Science & Technology's Foundry Institute

Industrial Advisory Panel

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Mr. P. Bradstock, Chief Executive, The Oxford Trust
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Professor B.L. Eyre, CBE, FREng, Chairman, Central Laboratory for the Research Councils
Mr. R. Malthouse, 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

Alumni Association Committee

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Dr. M. Burden, Technical Director, Dowty Aerospace Propellers
Sir David Cooksey, Advent Venture Partners.
Professor R.D. Doherty, Drexel University
Mrs E.A. Finch, Price Waterhouse Coopers
Dr. K.M. Fisher, Dowty Automotive
Dr. S. Flood, Powdrex Ltd (Committee Chairman) deceased during academic year
Mr. A. Geddes, Metal Agencies Ltd / Viohalco Group Greece
Mr. N.P. Gregory, Abingdon School
Mr. D.K. McLachlan, Tax Partner, Pricewaterhouse Coopers
Dr. K.A.Q. O'Reilly, Department of Materials, University of Oxford
Mr. C.G. Purnell
Professor G.D.W. Smith, FRS, Department of Materials, University of Oxford

Research Sponsors

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.

AEA Technology / Accentus
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Seagate Technology Ltd
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Teaching Company Scheme
Thai Government
The Royal Society
Toppan Printing Company
UKAEA
Wellcome Trust

Profiles of Academic Staff

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

Research, both experimental and modelling, on a range of polymer and polymer composite materials. Particular areas of interest include crystallinity and morphology, the relationship between processing and microstructure, surface characterisation and modification and polymer coatings.

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.

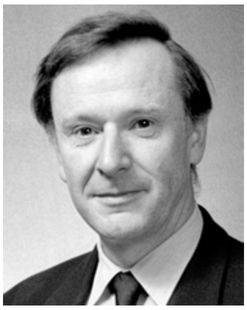
Dr. Roger Booker **Emeritus Reader in Electronic Materials**
Wolfson College **OCAMAC Senior Fellow**

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

Professor Andrew Briggs **Professor of Materials**
Wolfson College

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 **Professor of Materials**
St Cross College

Processing and properties of ceramic materials.

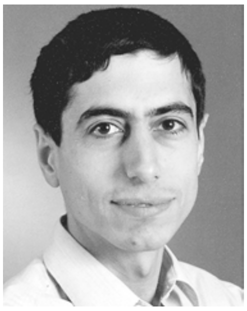
[Currently Director of the Leverhulme Trust]

Dr. David Bucknall **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 **Royal Society University Research Fellow**
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

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. 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. Patrick Grant **Reader in Materials Processing**
Linacre College **Director of OCAMAC**
Director of Faraday Partnership

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**

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

Dr. Chris Grovenor **Reader in Materials**
St Anne's College **Deputy Head of Department**

Applied superconductivity and the processing of electronic materials. Most 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. Recently, 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, 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

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, and quantitative imaging of defects.

Dr. Angus Kirkland **Leverhulme Senior Research Lecturer**
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.

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 nanostrctures (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. Study of size and shape distribution of quantum dots to develop a nanostructure diagram as a function of codeposition and growth parameters.

Dr. Peter Northover **Lecturer in Materials**
St Catherine's College **Practical Class Organiser**

Non-ferrous and precious metallurgy and metalwork in ancient and historical contexts and their experimental reproduction; engineering metallurgy of the industrial revolution; very long term stability of microstructures; 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.

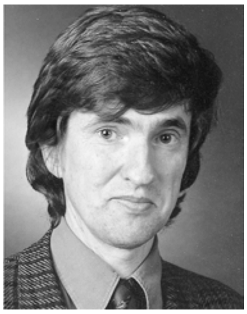
Professor Amanda Petford-Long C.Phys **Professor of Materials**
Corpus Christi College

The correlation of microstructural and magnetic or optical properties of thin films with applications in information storage. The main characterisation tool is TEM, including in-situ techniques to study magnetisation mechanisms (Lorentz microscopy) in magnetic thin films, and crystallisation and growth kinetics in optical and magnetic nanocomposite films.

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. Rosetta Plummer **Department Administrator**
St Edmund Hall

Responsible for the departmental finances, buildings, personnel management and provision of technical and secretarial services. Focal point for research agreements, development of the department's use of the Begbroke Science and Business Park, and services to industry.

Dr. Steve Roberts **Reader in Materials**
St Edmund Hall

Mechanical behaviour of materials, especially their response to surface deformation and the brittle-ductile transition. 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 **Head of Department**

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.

- Rosenhain Medal and Prize, 1991.
- Sir George Beilby Medal and Prize, 1985.

Dr. Ian Stone **Senior Research Fellow**

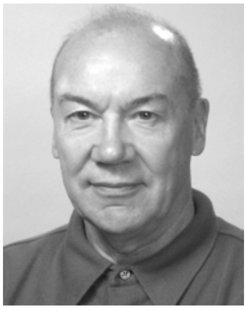
Processing-microstructure relationships in alloys and metal matrix composite systems. Evolution of microstructure during the spray forming process, grain growth in the semi-solid state, deformation behaviour of semi-solid alloys. Squeeze casting and rheocasting of wrought alloys. Manufacture and characterisation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

Professor Adrian Sutton FRS FInstP FIMMM FRSC CPhys CEng Professor of Materials
Linacre College

Theory and Simulation of processes within materials at the atomic and microstructural level.

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 **RAE Research Professorship in**
St Anne's College **Microanalysis and Structural Integrity**

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

Mechanical properties of ceramics and metals. Most research revolves around oxide ceramics, thermal residual stresses, neutron and X-ray diffraction, and superplastic metals. Current interests include the processing and mechanical properties of alumina matrix nanocomposites, residual stresses in thermally sprayed coatings, characterisation of cold worked microstructures using diffraction peak profile analysis, and projects on the superplastic forming and diffusion bonding of commercial alloys.

- 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 study crystallographic morphology of spherulitic structures, nucleation and crystallization, stabilization, degredation, electrical conductivity, fluorescence, diffusion, permeability, solubility and mechanical 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 **Royal Society University Research Fellow**
Corpus Christi College **Lecturer in Materials**

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

Physical properties of Li-Mg alloys

Dr. G. Taylor, Dr. M.E. Siedersleben, Professor S. Naito***

Thermal expansion coefficients and the values of elastic constants C11, C12 and C44 are being studied over the temperature range 4-300K for alloy compositions between 40 and 70at% magnesium. (*Honsel Werke Reichmetalle, Germany; **Kyoto University, Japan)

Fundamentals of cyclic deformation and fatigue crack initiation

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

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. Recent work concerns Si fatigued at elevated temperatures.(*Ecole des Mines, Nancy, France)(Funded by the Royal Society)

Measurement and development of residual stresses in coatings

*S. Saunders, Dr. R.I. Todd, Dr. J. Lord**

We are developing a robust method for measuring residual stresses in coatings both during deposition, and as they develop during simulated service. The method is based on the measurement of the curvature produced in coated substrates by the residual stresses. Although the basic method is well established, there is considerable uncertainty surrounding the assumptions used in interpreting the results. We are investigating these systematically using both commercial coating compositions, and model materials which can be selectively removed following deposition so that the effect of the deposition process itself on the stresses in underlying layers can be ascertained. The work is currently concentrating on thermally sprayed coatings, but the methodology developed may also be applied to other coating techniques. (*National Physical Laboratory) (Funded by EPSRC and NPL)

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 ~1600^{o}C. 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.

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, A. Other*, A.N. Other*

The project aims to formulate contimuum models of plastic flow in three dimensions, and to apply these to crack initiation and propagation in muti-phase materials. The models will be keyed to experimental studies of fracture nuclei and crack-tip plastic zones in steels with simplified microstrcutures. (*Oxford Centre for Industrial and Applied Mathematics) (Funded by EPSRC)

Brittle-ductile transitions in BCC metals

*T. Joseph, Dr. S.G. Roberts, Dr. S.L. Dudarev**

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

Core structure of screw dislocations in b.c.c. metals

Professor Sir Peter Hirsch

Isotropic elasticity calculations show that the symmetrical 3-fold dissociation of screw dislocations in b.c.c. metals is metastable. Yet atomistic computer calculations usually show 3-fold dissociated structures, dissociated mainly on {110} planes. Work is in progress to identify the basic physical reasons for the differences between the two approaches.

II – INTERMETALLICS

Mechanical properties of RuAl and (Ru,Ni)Al alloys

S.J. Pak, Dr. G. Taylor

The ruthenium aluminium system forms an intermetallic compound with the B2 structure at 50 % Al. In the main Ni can be substituted for Ru without change of structure and the solid-solution hardening adds considerable strength to the material. The mechanical properties are being studied by compression tests and transmission electron microscopy. 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.

Mechanical properties of CoTi based alloy single crystals

L. Zhang, Dr. M.L. Jenkins, 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 CoZr or 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.

Mechanical properties of lamellar TiAl and effects of purity and composition

*Dr. G. Taylor, Professor S. Naito**

Polysynthetically twinned crystals may be formed during growth of TiAl binary alloys depending on composition and growth conditions. A series of binary alloys with very high purity has been made for the study of mechanical behaviour and yield stress values over a range of temperatures. (*Kyoto University, Japan)

Formation of APB tubes in γ–TiAl

Professor Sir Peter Hirsch

Antiphase boundary tubes are a common feature of the deformation of γ–TiAl over a wide range of temperatures. A model previously proposed by the investigator for their formation is being developed in detail.

Simulation of weak-beam images of defects in γ–TiAl

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

Weak beam images of 1/2[112> edge dislocations in γ–TiAl are being simulated using the CUFOUR programme with a view to distinguishing between possible alternative structures of these defects. A model has been developed to explain the locked nature of these defects. (Funded by EPSRC)

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

S.J. Pak, Dr. M.L. Jenkins, Dr. G. Taylor

Single crystals of γ–TiAl are being grown with a [001] orientation from high purity alloys in the range 53.5-56 at%Al. They will be deformed in compression and also in tension over a range of temperatures to study the yield stress anomaly. Selected slices will be 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)

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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 collboration with Morgan Electro Ceramics)

Residual stresses and mechanical properties in oxide matrix nanocomposites

N. Wain, Dr. R.I. Todd

Preliminary results have shown that MgO/SiC nanocomposites have greatly improved strength and toughness compared to unreinforced MgO. The project aims to identify the mechanisms involved, with a focus on the large thermal residual stresses, in excess of the yield stress, which are to be expected in this system. The work will be extended to investigate the importance of such effects in other oxide matrix systems such as alumina/SiC. (Funded by EPSRC)

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

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

The project is aimed at use of alumina - silicon carbide ceramic nanocomposites in applications where wear and abrasion resistance are important. The project is focussed on the surface mechanical properties of sintered ceramic nanocomposites. There are two main aims - (a) to understand the mechanisms of their improved properties over normal alumina ceramics; (b) to produce materials usable in real industrial applications. This project is in collaboration with Morgan Matroc. (Funded 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 a single-crystalline, 3-D networks, giving unusual properties. (*In collaboration with the Ioffe Physical-Technical Institute, St Petersburg, Russia, supported by the Royal Society)

PLZT microstructures for high strain piezoelectric applications

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

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)

Structure and properties of 'Hardide' coatings

*D. Di Maio, Dr. S.G. Roberts, Dr. C.R.M. Grovenor, Y. Lakhotkin**

A new class of ultra-hard coatings has been developed. The project will investigate their structure and properties. (*Hardide Ltd.)

Environmental effects on surface damage in float glass

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

The project will use 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)

II - BIOMEDICAL MATERIALS

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)

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)

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.

Mechanical properties of biocomposites

D. Gotora, Dr. J.T. Czernuszka

Composites based on natural systems are being made and their dynamic mechanical and fracture response determined. New models of how this class of materials deform are being formulated. (Funded by the Rhodes Trust)

Macro-assembled spheres of apatite

O. King, S. Wilkinson, Dr. J.T. Czernuszka

Lipid spheres are being coated with apatite which are then deposited on to metallic surfaces. We have hierarchical control of the macro-assembly on 5 length scales. The liposomes are being filled with pharmaceutical agents, such as anti-biotics and growth factors. (Funded by Wellcome Trust, EPSRC)

Tissue Engineering of Heart Valves

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

Scaffolds for the tissue engineering of heart valves are being fabricated using our novel fabrication route. The scaffolds are seeded with interstitial (and other) cells and their perfomance monitored. (* Begbroke Technolgy Centre, ** Harefield Hospital)

In vitro approaches to bone formation

Dr. J.T. Triffitt, Dr. J.T. Czernuszka, E Sachlos*

Processes are being developed that encourage bone formation on a laboratory scale. The control and manipulation of osteoblasts is of the utmost importance. (*Nuffield Department of Orthopaedic Surgery) (Funded by EPSRC and in collaboration with MRC Bone Research Lab.)

In situ formation and electrodeposition of active coatings

S. Wilkinson, O. King, Dr. J.T. Czernuszka

Electric fields are used to regulate the precipitation rates of sparingly soluble solids. Biologically active coatings have been fabricated and we are now extending the process to other systems. (Funded by EPSRC)

Tissue Engineering and three-dimensional scaffolds

E. Sachlos, Dr. J.T. Czernuszka, Professor Z.F. Cui, Professor B. Derby***

A three dimensional printing method is being developed to promote the alignment, proliferation and differentiation of cells. The project will examine various cell types. (*Dept of Engineering Science; **UMIST)

An improved bone-implant interface

A. Walpole, 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. (* Faculdade de Engenharia ElŽtrica e de Computa□‹o, Universidade Estadual de Campinas, Brazil)

Modelling phospholipid monolayers at the alveolar interface

Dr. I. Gentle, Dr. D.G. Bucknall*

Phosphatidylcholine molecules play an important role in the action of natural lung surfactants by supplying lipids to the alveolar monolayer. The exact mechanism for this process remains uncertain. Using self-assembling layers in a Langmuir-Blodgett apparatus, surface pressure, neutron reflectivity and Brewster angle microscopy studies of the compression-expansion cycles of these systems is being used to investigate the physiological behaviour within a lung. (*Department of Chemistry, Queensland University) (Funded by Australian Government)

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 are other similar congenital deformities. (* Nuffield Dept of Surgery, **Dept of Plastic Surgery)

Three Dimensional Scaffolds for Tissue Engineering

E. Sachlos, Dr. J.T. Czernuszka, Professor Z.F. Cui, Professor B. Derby**, N. Reis***

Scaffolds are being fabricated using novel ink jet printing techniques. The mesostructure is being tailored to encourage vascularisation and subsequent tissue incorporation. The nanostructure, microstructure and mesostructure are all being tailored to optimise the degradation rate and mechanical properties. (*Dept. Engineering Science, University of Oxford; **Manchester Materials Science Centre) (Funded by EPSRC and Boddosaki Foundation)

Understanding Bioselective Surfaces and their Medically Relevant Ligands

*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)

III - POLYMERS

Direct-write microlithography in polymers and glass using MeV ion microbeams

Dr. G.W. Grime, M.H. Abraham, I. Gomez-Morilla,*

The low scattering of MeV ions in solids means that the ~1 micron spatial resolution of a focused proton beam is maintained over a long range (typically 60 microns in silicon at 2 MeV). High aspect-ratio structures have been fabricated in PMMA and photo-sensitive glass. Grooves 1 micron wide and 100 microns deep can be formed, and more recent work has produced miniature (100 microns diameter) gear wheels and turbines with angled blades in PMMA. Structures have also been formed in photo-sensitive glass, and preliminary results show that it is possible to form buried waveguides in glass.(*University of Surrey)(Partly funded by the British National Space Agency)

Ion beam lithography

Dr. G.W. Grime, I. Gomez-Morilla, Dr. D.G. Bucknall*

The use of medium energy ion beams is being investigated as an alternative method of producing high aspect ration topographic patterning. The use of both patterned masks as well as micro-focussed probes is being investigated to produce not only 2D as well as 3D structures. (* Department of Physics, University of Surrey)

Gloss of polymers

Dr. H.E. Assender

The gloss of a material is a measure of the specular reflectance of light from the surface. The gloss depends upon the roughness of the surface. AFM examination of a range of polymer surfaces is being applied to allow quantitative analysis of the roughness to link the topography of a surface to the measured gloss. Related scanning force microscopy techniques, such as UFM, are used to monitor the morphological origin of the roughness.

Thin film properties of macrozwitterions under the influence of an electric field

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

Macrozwitterions have slightly different properties in thin film compared to the parent unfunctionalised homopolymer, due to segregation of the oppositely charges end groups. The molecular structure and orientation can be drastically altered by application of external fields when in the melt. This project is studying the effects of applying an external field to the polymer morphology within these thin films, not only to understand the orientation behaviour in restricted geometry but also to be able to manipulate the film properties. (*IRC in Polymer Science and Technology, Durham University)

Real time studies of polymer interfaces

Dr. D.G. Bucknall, Dr. S.A. Butler, Professor J.S. Higgins***

This project is developing the methodology, techniques and apparatus required to conduct neutron reflection experiments in real time. The technique has been applied to investigate the diffusion of oligomers and plasticisers into polymers and to study the subsequent dissolution of the polymer films. This is the first time that such measurements have been successfully carried out in real time, providing new information and insight into the processes involved. (*Department of Chemistry, Cambridge University; **Department of Chemical Engineering, Imperial College) (Funded by EPSRC)

Structure and dynamics of polyrotaxanes

*Dr. D.G. Bucknall, Professor H.W. Beckham**

Polyrotaxanes are a novel polymer which consist of macrocycles treaded onto the polymer chain. The incorporation of these rings on the chain can have a dramatic effect on the physical properties as observed by its structure and dynamics. Using a combination of solid state NMR, quasi-elastic and small angle neutron scattering, and X-ray diffraction the molecular basis for these physical changes are being investigated. (*Department of Textile and Fiber Engineering, Georgia Institute of Technology) (Funded by NATO)

Effects of molecular architecture on polymer interdiffusion

Dr. D.G. Bucknall, Dr. N. Clarke, Dr. J.H.G. Steinke**, Professor J.S. Higgins****

Although the idea of polymer diffusion via reptation is well understood for linear polymers, the same is not so true for non-linear polymers. This project is studying the effect of molecular architecture on the diffusion process for a set of chemically identical polymers, and using this model system to interpret the behaviour under the framework of the reptation model. (*Department of Chemistry, Durham University; **Department of Chemistry, Imperial College; ***Department of Chemical Engineering, Imperial College)

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 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.

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.

Luminescent Conjugated Polyrotaxanes

Dr. H.L. Anderson, Dr. D.G. Bucknall, Dr. F. Cacialli**, Professor R.H. Friend***

Conjugated polymers have many potential applications, particularly as organic semi-conductors and electroluminescent display materials. We are developing a way of improving the luminescence, stability and processability of these polymers by insulating with threaded macrocyclic rings to form polyrotaxanes. This work represents the first use of rotaxane formation to control the optoelectronic properties of a conjugated polymer chain, by isolating, insulating and encapsulating it. These new materials will provide fundamental insights into the behaviour of conjugated polymers by controlling inter-chain separation, so blocking short-range inter-chain processes. (*Dyson Perrins Lab., Oxford University; **Cavendish Lab, Cambridge University) (Funded by EPSRC)

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)

Nano-structures derived from polyrotaxanes

Dr. D.G. Bucknall, Professor H.W. Beckham, H.L. Anderson***

Polyrotaxanes are polymers which have been threaded by macrocyclic rings, which can have a dramatic effect on the properties of the polymer. We are exploring the use of polyrotaxanes as a synthetic route to forming molecular scale devices which can mimic the behaviour of switches, magnetic memory disks and circuit wiring. Polyrotaxanes have potential to be exploited in a number of these molecular scale devices by manipulation of the polymer and macrocycle chemistry. (*Department of Textile and Fiber Engineering, Georgia Institute of Technology; **Dyson Perrins Lab, Oxford University)

Unstable polymer-polymer interfaces

*Dr. D.G. Bucknall, Dr. M. Sferrazza**

The width of an interface between immiscible polymers is determined by the Flory-Huggins parameter. However, when measured using techniques such as neutron reflectivity the interfacial width measured is larger than expected due to thermally excited capillary waves. The amplitude of these capillary waves and therefore the magnitude of the contribution to the measured interfacial width is logarithmically dependent on the film thickness. We are studying the behaviour of thin films where the film thickness is of order of the chain dimensions (geometrically confined), and therefore similar to the capillary wave amplitude. This can lead to dewetting occurring. As expected this can be altered by altering the interaction between the polymers and the substrate, surprisingly though the unstable films become metastable when mechanically confined. This Part II project aims to understand the mechanism of dewetting and the role played by capillary waves in mechanically confined thin films. (*Department of Physics, Surrey University)

Mechanisms of Glass Transition of Polymer Thin Films

T. Kanaya, I. Tsukushi**, Dr. D.G. Bucknall*

Polymer thin films show some interesting but unusual features. One of them is the glass transition temperature, Tg, of these thin films is very different from that of the bulk. We are studying the behaviour of polymer thin films to understand this behaviour within the context of a new glass transition mechanism recently proposed. (*Institute of Chemical Research, Kyoto University; **CIT, Chiba, Japan) (Funded by Japanese Research Council)

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.

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. C. Borman**

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. 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.

Microfluidic phase mixing and demixing

Dr. D.G. Bucknall, Dr. J. Yeomans, Professor A. Balazs**, C. Vasa*

Phase mixing and demixing of binary mixtures is being investigated in confined systems where the volume of the fluid is potentially as little as a few microlitres. Theoretical models have been established to simulate fluid mixing of oligomer blends and binary fluids when confined between chemically heterogeneous surfaces. These models will be tested experimentally using microfluidic devices and then the system extended to study demixing processes. (*Department of Theoretical Physics, Oxford University, **Department of Physics, Pittsburgh University, USA)

Influence of heterogeneous surfaces on polymer thin film behaviour

Dr. D.G. Bucknall, Dr. H. Zhang, Professor G.A.D. Briggs

Using a number of non-conventional lithography techniques for chemical and topographic patterning of solid surfaces, the behaviour these surfaces have on thin polymer films is being studied. In particular the role played by incompressible solid capping layers on the polymer is being investigated in order to drive the polymer film to form highly anisotropic topographic features. (Funded by EPSRC)

IMAGE-IN: Improved Ink Jet Printing by Control of Ink Media Interactions

Dr. D.G. Bucknall, Professor G.A.D. Briggs, Dr. A. Dupuis, Dr. J. Leopoldes, Dr. S. Wilkins, Dr. J. Yeomans, members of AGFA-Gevaert, Ardeje, Coates Electrographics, Dotrix, Teich and Universite Joseph Fourier.

This project addresses industrial ink jet printing technology with a strong innovative approach of bringing together a pan-European partnership of expertise along the entire technological and scientific chain of inks, media, and hard- and software integration, underpinned by a strong scientific research programme. The project uses a holistic approach to the scientific understanding of commercial and industrial ink jet technology from ink composition, through ink jet ejection, surface treatment methods and subsequent ink-substrate interaction to final print quality characteristics. (see www.imagein.org for further details)

Behaviour of model ionomer solutions

Dr. D.G. Bucknall, Dr. B. Gabrys, Professor T. Kanaya**, Dr. W. Smith****

The solution behaviour of nano-assemblies of telechelic polymers (model systems for ionomers and polyelectrolytes) is being studied using complementary light, X-ray and neutron scattering, combined with molecular dynamic simulations. The concentration dependence of the telechelic polymer morphology and dynamics will be studied not only theoretically but also by development of time-resolved static scattering experiments. (* Department of Applied Mathematics, Open University, ** Institute of Chemical Technology, Kyoto University, *** Daresbury Laboratory)

Structure and properties of silk

*Dr. J.T. Czernuszka, Professor C.Viney**

A variety of spider and insect silks are being characterised by transmission electron microscopy/diffraction. The aim is to correlate microstructure to mechanical properties, in the context of silk evolution.(*Heriott-Watt University)

Long range ordering of block copolymer

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

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)

Polymer-Plasticiser Diffusion

Dr. D.G. Bucknall, Dr. S.A. Butler, Professor J.S. Higgins***

The ingress and egress of plasticisers in polymer thin films is being studied using detailed depth profiling techniques (neutron scattering and dynamic SIMS) coupled with microscopic IR mapping. Detailed analysis of the evaluation of the plasticiser concentration profile and interfacial profile is being mapped and compared to diffusion theories of small molecule penetrants in high molecule weight matrices. (* Department of Chemical Engineering, Cambridge University, ** Department of Chemical Engineering, Imperial College).

IV - PHOTOVOLTAIC MATERIALS

Deposition and characterisation of nano-porous conducting oxide films

Z. Xie, Dr. B.M. Henry, Dr. 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 uses sputtering, sol-gel and anodising to fabricate thin films with controlled structure. The electrical properties of the films, and their compatibility with new functional polymers, is being studied and correlated with the nanostructure of the films investigated by SEM, TEM and AFM. (Supported by the Toppan Printing Company Ltd.)

Modelling photovoltaic devices

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

We will identify an simulate the key elements in the operation of a polymer/TiO2 photovoltaic device. 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 Priniting Company)

Synthesis of novel organic materials for photovoltaic devices

Dr. G.R. Webster, B. Lochab*, 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 architechtures and improved device performance. (*Dyson Perrins Laboratory, Oxford University)(Supported by the Toppan Printing Company Ltd.)

Modelling of polymer-conducting oxide photovoltaic devices

Dr. V. Burlakov, Professor A.P. Sutton

Photovoltaic devices comprising photo-sensitive conducting polymers and conducting amorphous oxides are being designed, built and characterised as part of a second collaboration with The Toppan Printing Company. In this project the devices are being modelled at a continuum level to elucidate optimal device morphologies, and to develop equivalent circuit models to enable experimental I-V curves to be interpreted. One of the principal goals of the modelling is to identify the critical materials parameters limiting the efficiency of the photovoltaic devices.(Supported by the Toppan Printing Company Ltd.)

The optoelectronics of organic photovoltaic materials.

A. Barkhouse, K. Kawata, Dr. M.J. Carey, Dr. H.E. Assender

This work focusses 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 Toppan Printing Company Ltd.)

Device manufacture and characterisation of organic photovoltaic materials

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

An organic-inorganic nanocomposite photovoltaic material is being designed and characterised. This work seeks to characterise the various materials components in the device, with particular emphasis on the organic components and interfaces, and to improve the device manufacturing processes for lab-scale testing. (Supported by the Toppan Printing Company Ltd.)

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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.

Grain boundary properties in Tl-2212 films

S. Speller, C.J. Dark and Dr. C.R.M. Grovenor

The properties and structure of grain boundaries in Tl-2212 thin films are being studied to correlate structure with critical current performance. Both artificial and natural grain boundaries are being grown on LaAlO3 and MO substrates, and doping of the boundaries to improve properties is also being attempted. (Funded by EPSRC)

Development of novel metallic substrates for superconducting tapes

R.M. Whiteley, Dr. C.R.M. Grovenor

The thermal/mechanical properties of silver and silver alloy substrates have investigated to identify the most promising material for use in high temperature superconducting tapes. High quality <110> textured Ag substrates are being produced and supplied to collaborators in the USA and Europe for the deposition of REBaCuO superconductor layers by a wide range of techniques. (In collaboration with the Department of Metallurgy, University of Cambridge)

Synthesis and microstructure of MgB2 powders and wires

S. Haigh, Dr. H. Wu, C.J. Salter, Dr. C.R.M. Grovenor, Dr. P. Kovac***

MgB2 is a most promising new superconducting material for high current applications at temperatures below 30K. We are studying new methods for the chemical synthesis of high quality 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)

Microstructural characterisation of superconducting materials

Dr. H. Wu, S. Speller, C.J. Dark, S. Latif, Dr. 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, XRD texture analysis and orientation imaging microscopy techniques are being used to study the key microstructural features - especially the grain boundary structure and properties. (Funded by EPSRC and in collaboration with Oxford Instruments and University College London, and University of Coventry*)

Fabrication of thin films of Tl-2212

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

Sputtering and post annealing processes are being used to deposit thin films up to 3 inches in diameter of Tl-based superconducting ceramics and buffer layers. 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 substrates are also being used to achieve off axis growth for specific device designs. The aim is produce optimised high Jc/low Rs materials for a wide range of practical applications. (Funded by EPSRC and in collaboration with Department of Physics, University College London, Department of Engineering Science*, Oxford, Department of Metallurgy and IRC in Superconductivity, University of Coventry**)

Development of electroepitaxy as a novel method for the production of textured metallic substrates for superconducting tapes

R.M. Whiteley, Dr. C.R.M. Grovenor, Dr. J.M. Sykes

We have recently demonstrated that electrodeposition of metallic layers on a textured substrate is a powerful way of growing epitaxial buffer layers of the kind required in second generation high temperature superconducting tapes. We are currently studying the deposition of Ag/Ni and Ag/diffusion barrier/Ni layer combinations in order to demonstrate the compatibility of these structures with in-situ deposited superconducting layers from collaborators in Germany and Cambridge. At the same time, the fundamental processes that operate in the phenomenon of electroepitaxy are being investigated. (In collaboration with Department of Metallurgy, University of Cambridge and Theva GmbH)

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

M. Korsah, Dr. H. Wu, S. Speller, C.J. Dark, Dr. 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 challange of the project, and requires a very detailed understanding of nucleation nad growth processes in these films. (Funded by EPSRC and in collaboration with University College London and University of Coventry*)

II - SEMICONDUCTOR MATERIALS

Quantum wires and dots

Dr. J.L. Hutchison, F. Ito, X. Chen, Professor P.J. Dobson, R.N. Taylor, 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,; **Nanox Ltd.) (Funded by EPSRC and Nanox Ltd.)

Quantum dots

Professor V. Baranauskas, Dr. P.R. Wilshaw

A novel technique for producing quantum dots is being investigated which uses porous alumina as a template their size and distribution. The structures are being characterised by AFM, SEM and TEM.

Room temperature light emission form silicon

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

Different dislocation structures produced in silicon are being investigated using cathodoluminescence with a view to producing devices which emit at room temperature. (*Gatan, UK; **MEMC, Italy)

Secondary electron mapping of doped regions in semiconductors

Dr. M.R. Castell, Dr. A.J. Wilkinson, 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. (Funded by The Royal Society)

Impurities and dislocations in Si wafers

J. Murphy, A. Giannattassio, 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 is being studied. In particular the diffusivity and effect of H on diffusivity in the range 350-700ºC is being investigated together with the locking of dislocations by impurities and the mechanism by which precipitates weaken wafers. One of the aims of the project is to understand impurity-defect interactions so that stronger Si wafers may be manufactured. (*MEMC, Italy) (Funded by MEMC)

Investigation of strain distributions in semiconductors

*Dr. A.J. Wilkinson, Dr. C. Tager-Cowan**

A technique for probing local elastic strain fields using electron back scatter diffraction patterns has been developed. It is being used in conjunction with electron channelling contrast imaging to characterise local strain and defect distributions in semiconductor materials and devices. Recent work concerns characterising strain distributions in epitaxially laterally overgrown GaN films, in collaboration with (*University of Strathclyde) (Funded by The Royal Society)

Electron field emission from dielectric films

E. Kirkby, 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.

III - MAGNETIC MATERIALS

Microstructure and magnetic structure of spin-valves and exchange-couples

Professor A.K. Petford-Long

The microstructure and magnetisation reversal mechanisms of spin-valve devices and exchange-couples with applications in information storage technology are being studied at high spatial resolution using electron microscopy, for correlation with their giant magnetoresistive properties. (In collaboration with Seagate Technology) (Funded by EPSRC and Seagate Technology)

Composite magnetic nanoparticle systems

A. Eggeman, 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. (*Academic Director of the Oxford University Begbroke Science Park, **Johnson Matthey) (Funded by EPSRC and Johnson Matthey)

Spin-tunnel junctions based on magnetic layered films

Professor A.K. Petford-Long, G. Hodge, 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. (*Hewlett-Packard Labs.) (Funded by Hewlett-Packard Labs. and EPSRC)

MBE growth of spin-valve structures and exchange-biased layers

*Y-S. Choi, Professor A.K. Petford-Long, Dr. R.C.C. Ward**

The MBE system in the Clarendon Laboratory is being used to grow epitaxial spin-valve structures and 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. (*Clarendon Laboratory, Oxford) (Funded by EPSRC)

Studies of patterned magnetic thin films

N.W. Owen, 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)

IV – QUANTUM INFORMATION PROCESSING

Nanoelectronics at the Quantum Edge

Professor G.A.D. Briggs, Dr. S.C. Benjamin, Dr. R. Taylor, Professor N.F. Johnson*, Professor D.G. Pettifor, Dr. D. Hasko**, Dr. D.A. Williams***, Dr. A. Ardavan**

Oxford and Cambridge Universities are working together with Hitachi Europe Ltd to produce radically new devices for future computing. The project brings together research in physics, chemistry, materials science and electronics engineering to make prototype structures for advanced conventional computing and for the new field of quantum computing. Quantum computation is potentially the most innovative area that can be addressed within the field of nanotechnology, embracing nanofabrication, molecular nanotechnology, and atomic and molecular manipulation and assembly. Tremendous progress has been made in the fundamental theory of quantum information, and there is now a global race to find a practical technology for quantum computing. Our initial strategy will be to develop the three most promising solid-state nanotechnologies: a molecular approach, an all-optical approach involving self-assembled quantum dots, and a single-electron approach based on nanolithography. Having determined the 'winner' for quantum computing, and having also evaluated the potential for revolutionary classical computing, we shall then focus on creating prototype circuits. These will embody a radically new global addressing architecture, which enormously reduces the number of wires and offers very significant advantages both in terms of the fundamental physics and in terms of the practical nanofabrication. By the end of the project we shall have realized a small quantum circuit suitable for subsequent development into a full quantum computer. See www.nanotech.org for more information. (Funded by DTI Foresight LINK Award through EPSRC and Hitachi Europe Ltd)

Physical embodiment of qubits

M.R. Austwick, Dr. A. Ardavan, Professor G.A.D. Briggs*

We shall investigate the physics of candidate systems for embodying qubits in a solid state quantum logic gate. (* Clarendon Laboratory)

Assembly of Molecular Arrays in Single-Walled Carbon Nanotubes

A. Khlobystov, S. Boden, M. Austwick, Dr. K. Porfyrakis, G. Morley, Dr. A. Ardavan, Dr. J. Dennis**, Professor G.A.D. Briggs*

A central part of the project is the engineering of molecular arrays inside single-walled carbon nanotubes. The nanotube can encapsulate magnetically or optically active molecules, such as endohedral fullerenes and other organic or organometallic molecules. The nanotube will also act as a channel of communication between the encapsulated molecules within the 1D array, which will allow design of new carbon-based hybrid materials exhibiting unusual magnetic, mechanical and electronic properties. (*Department of Physics; ** Department of Chemistry, Queen Mary College, London) (Funded by EPSRC Foresight LINK Project, DTI and Hitachi Europe).

STM/STS of nanotubes

D. Leigh, Dr. J.H.G. Owen, Dr. A. Ardavan, Professor G.A.D. Briggs*

We aim to use Scanning Tunnelling MIcrosocopy (STM) and Scanning Tunnelling Spectroscopy(STS), in conjunction with other spectroscopic techniques, to explore the physical and electronic structure of so-called "peapod" nanotube structures; that is, nantoubes which contain fullerenes, which may themselves contain atomic species such as Y, Ce, or even N. STS is especially important to this work, as the electronic structure of the nanotube, and therefore the interactions between the endofullerenes and the encapsulating nanotube, depends upon its size and chirality. Current experiments are being conducted on graphite and gold substrates, suitable for ambient imaging, but future experiments will be conducted in UHV conditions, so as to allow the use of UPS and XPS to characterise the peapods' electronic structure as well as STM/STS. (Funded by EPSRC Foresight LINK Project, DTI and Hitachi Europe).

A Quantum Field Theoretical Approach to Decoherence of Quantum Dot Registers

Dr. J.H. Reina, Dr. S.C. Benjamin, Professor G.A.D.Briggs, Dr. B.W. Lovett, A. Nazir*

The aim of this work is to investigate how, when memory effects are taken into account, environmental decoherence affects the unitarity of the quantum evolution of an optically excited quantum dot (QD) molecule recently proposed by us as a hardware system for quantum computation. Given that the associated energy scales of the qubit-qubit interactions are on the sub-picosecond time scale, such a non-Markovian description becomes crucially important in the understanding of the stability and scalability of the envisaged QD quantum computer. (*Clarendon Laboratory, Department of Physics) (Funded by EPSRC Foresight LINK Project, DTI, Hitachi Europe and The Royal Society).

Bio-molecular Quantum Computation

Dr. J.H. Reina, Dr. S.C. Benjamin, Professor G.A.D. Briggs, Dr. B.W. Lovett, A. Nazir*

This study aims at implementing the use of the resonant transfer of excitons in complex bio-molecular systems (e.g., the purple bacteria Rhodospirillum molischianum) for quantum computing purposes. We have performed some calculations that support the feasibility of such an approach, but this study is still in progress and needs further exploration.(*Clarendon Laboratory, Department of Physics) (Funded by EPSRC Foresight LINK Project, DTI, Hitachi Europe and The Royal Society) (In collaboration with Hewlett Packard Laboratories Bristol).

Theory of Quantum Computing with Excitons in Quantum Dots

Dr. B.W. Lovett, Dr. J.H. Reina, A. Nazir, Dr. S.C. Benjamin, Professor G.A.D.Briggs,*

The strength and nature of the interactions between excitons in self assembled quantum dot structures will determine how suitable they are as quantum information processors. We have been performing theoretical investigations into these interactions and have recently shown how to optimize such a molecule so that simple quantum logic can be performed. We have proposed two alternative possibilities: one which uses coupling to a light field to control the quantum state of the molecule, and another which uses the internal interactions to do this. See http://www.nanotech.org/research/theory/QDrelated/index.html for more details. (Funded by EPSRC Foresight LINK Project, DTI, Hitachi Europe and The Royal Society) (In collaboration with Hewlett Packard Laboratories Bristol)

ESR Study of Carbon Nanostructures for Quantum Computing

G. Morley, Dr. A. Ardavan, Professor G.A.D. Briggs*

Molecules of N@C60 have an exceptionally sharp ESR signalÊcorresponding to long-lived electronic spin states. The suitability of theseÊstates 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. See www.nanotech.org (*Department of Physics) (Funded by EPSRC Foresight LINK Project, DTI and Hitachi Europe).

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D. Processing

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

Dr. J. Mi, Dr. I.C. Stone, Dr. 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)

Rapid spray formed tooling

T. Rayment, Dr. S. Duncan, Dr. P.S. Grant*

Electric arc spraying of liquid steel droplets onto shaped substrates is being investigated for the rapid manufacture of dies for stamping/pressing tools for a wide range of applications. Lead times are several times faster than for conventionally machined dies and tooling. Research focuses on closed loop feedback control of residual stresses, simulation of shape evolution and microstructural characterisation. (*Department of Engineering Science) (Funded by EPSRC, Sulzer Metco and Ford Motor Co.)

DC and shape casting of wrought Al alloys

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

Novel manufacturing routes for Al products

C.D.J. Manson-Whitton, Dr. K.A.Q. O'Reilly, Dr. M. Clinch, Dr. W. Hepples*, Dr. H. Holroyd**

Novel manufacturing technologies are being investigated for the manufacture of Al alloy products.(*Luxfer Group) (Funded by The Royal Commission for the Exhibition of 1851 and Luxfer Group Ltd.)

Spray formed Al-Li and 7XXX alloys alloys for airframe applications

Dr. S. Hogg, Dr. I.G. Palmer, Dr. 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 and 7XXX 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).

Multicomponent alloys

*K-B. Kim, Dr. P.J. Warren, Professor B. Cantor**

Solidification of multicomponent alloys often results in complex microstructures consisting of a mixture of stable and metastable phases. These microstructures or individual constituent phases can exhibit a range of unusual and desirable properties such as magnetic, elastic or structural. This project is working near the centre of several different five and six component phase diagrams, outside the regime currently accessible by thermodynamic modelling. (*University of York)

Mechanical properties and microstructural evolution of semi-solid alloys

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

Viscometry methods are being developed in order to measure the mechanical response of semi-solid slurries. The results are being used to determine semi-solid constitutive laws, and are being applied to a variety of metallurgical manufacturing processes, particularly for Al alloy automotive components. (*University of York)

Carbon fibre reinforced magnesium

*M. Russell-Stevens, Dr. R.I. Todd, P. Schultz**

Microstructural, residual stress and mechanical properties of long fibre carbon fibre reinforced magnesium alloys manufactured by squeeze casting are being investigated. (*Leichtmetall Kompetenzzentrum Ranshofen) (Funded by EPSRC)

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. (Funded by JIF in collaboration with Luxfer Group)

Squeeze casting and semi-solid processing of Al alloys

*C.D.J. Manson-Whitton, Dr. I.C. Stone, Dr. K.A.Q. O'Reilly, Professor B. Cantor**

An UBE 350 tonne squeeze casting and semi-solid processing machine is 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. (Funded by JREI and Luxfer Group)(*University of York)

Manufacture and characterisation of nano-quasicrystalline aluminium alloys

M. Galano, Dr. F. Audebert, Dr. I.C. Stone, Professor B. Cantor***

Al-base nanocomposite materials containing high volume fractions of quasicrystalline dispersoids are being produced by rapid solidification techniques. Particular emphasis is being placed on the dependence of alloy composition on the ability to form the quasicrystalline phase during quenching. This project is partly within the framework of an EU Research Training Network with 9 European partners (www.materials.ox.ac.uk/nano-al) (*University of Buenos Aires; **University of York) (Funded by EU and British Embassy Korea S&T Fund)

Spray formed silicon-aluminium alloys for electronic packaging applications

A. Lambourne, Dr. P.S. Grant

Alloys containing up to 70wt%Si are being manufactured by spray forming. These alloys offer a unique combination of low thermal expansion, high thermal conductivity and low density, and are investigation for electronic package thermal management applications in the avionics, satellite and other industries. The research concerns the characterisation of the key mechanical and microstructural properties of Al-70Si; the optimisation of spray forming; and to enhance alloy properties by ternary alloy additions. (In collaboration with Osprey Metals Ltd).

Control of temperature during vacuum plasma spraying

Dr. 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).

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, and will demonstrating the benefits of melt conditioning on (i) the manufacture of thin walled, high integrity automotive sand and die castings; and (ii) the selection of preferred intermetallic phases during DC casting. (* N-Tec Limited) (Funded by TCS and 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)

Measurement of cleanliness of molten magnesium alloys

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

Based on a proprietary technique, a method is being developed for the measurement of the cleanliness of molten magnesium alloys. (*N-Tec Ltd) (Funded by the Chevening Technology Enterprise Scholarship)

Reliable compact capacitors for aerospace applications

*C. Hinchliffe, Dr. V. Suvorov, Dr. C. Johnston, Dr. 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,)

Nodal optimisation in truss structures

Ms S. Panteny, Dr. 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.)

Advanced materials for plasma facing components (PFC) in fusion devices

G. Thomas, Dr. 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 contraints 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, minimimum porosity and surface roughness, etc. Some material combinations are novel and offer particular challenges for processing technologies. (Funded by UKAEA)

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

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

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).

The role of secondary intermetallic phase selection on hot tearing of aluminium alloys

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

Many Al alloys suffer from hot tearing (cracking) during casting due to high thermal stresses developed during solidification. The type, size and morphology of intermetallics formed during the final stages of solidification can affect hot tearing and that correct manipulation may lead to reduced hot tearing tendency. In this project, the morphology of the ‡-Al dendritic structure and the selection of secondary Al-Fe-Si phase intermetallics of an aluminium alloy are being controlled, and their influence on the mechanical properties of the alloy at very low solid fraction are being measured. (Funded by EPSRC)

Melt cleanliness in direct chill (DC) casting of 6xxx series aluminium alloys

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

Due to the presence of Fe and Si as impurities, Al-Fe-Si intermetallic phases form during DC casting of wrought Al alloys and have a marked effect on down stream formability by processes such as extrusion. Oxide films and inclusions entrained in molten Al alloys can influence the nucleation of these secondary intermetallics. Using techniques for the control and measurement of melt cleanliness, the aim of this project is to understand the role of oxide inclusions on secondary intermetallic phase selection.

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E. Phase Transformations, Surfaces and Interfaces

I - PHASE TRANSFORMATIONS

One-dimensional crystal growth inside single-wall carbon nanotubes

*Dr. J.L. Hutchison, Dr. J. Sloan, Dr. A.I.Kirkland, R. Carter, A. Vlandas 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)

Atomic scale studies of solute distributions at grain boundaries and interphase interfaces

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

The objective of this work is to understand how solute segregation to interfaces inhibits grain boundary migration and affects the kinetics of solid-state phase transformations. Atomic-scale analysis of solute segregation in the 3-dimensional atom probe will be combined with computer modelling using ThermoCalc/DICTRA.

The use of scanning calorimetry to investigate microsegregation in binary and multi-component alloys

E.C. Kurum, Professor J.D. Hunt

Experimental work on a novel scanning calorimeter is being used to study microsegregation in binary and multi-component alloys. The initial heating of twin-roll cast material will be used to investigate microsegregation during rapid solidification. The results are compared with the multi-component microsegregation model being developed with the group. (*Alcan International Research Laboratories) (Funded by EPSRC and Alcan International Research Laboratories)

Structure and crystallisation kinetics of optical and magnetic nanocomposites

J-P. Barnes, Professor A.K. Petford-Long, Dr. R. Serna, R.C. Doole,*

The effect of metal particle size and morphology on the ultrafast non-linear optical properties of nanocomposite materials is being studied. In-situ TEM annealing is being used to understand the kinetics of the crystallisation process. (*Institute of Optics, CSIC, Madrid, Spain)(Funded by EPSRC, British Council and Chinese Government)

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?

Cyclic phase transformations

*I. de Ardo, Dr. K.A.Q. O'Reilly, Professor B. Cantor**

The effect of temperature cycling is being investigated on the melting, solidification and solid state phase transformations in pure metals, alloys and amorphous materials using a novel calorimetric technique and TEM to determine kinetics of phase transformations. (*University of York)

II - OXIDATION AND CORROSION

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 (up to 1mm) and so normally, destructive methods such as sectioning are used to characterise the layers. The technique developed here uses a micro-focused 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 Oxford Scanning Proton Microprobe. The region of the surface removed by the laser beam is typically less than 500mm diameter and so, by comparison with other sampling techniques, the effect on the appearance of an object is minimal.(*University of Surrey)

Study of anti-corrosive paints by scanning acoustic microscopy and scanning Kelvin probe

Dr. B. Reddy, Dr. J.M. Sykes, Professor G.A.D. Briggs

The process of coating breakdown and adhesion loss is being examined by combined use of scanning acoustic microscopy and scanning Kelvin probe. The influence of metal-coated substrates, anti-corrosion pigment type and other coating variables is being determined.(Funded by EPSRC)

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)

Corrosion protection of metal packaging by organic coatings

M. Doherty, Dr. J.M. Sykes, Dr. H.E. Assender

The influence of barrier and other properties of polymer coatings on corrosion of food cans is being examined. Permeation and electrochemical measurements are supplemented by adhesion studies using scanning acoustic microscopy and potential mapping by scanning Kelvin probe. (Funded by EPSRC and in collaboration with Crown Cork and Seal)

The origin of corrosion in coated metal packaging containers

G. Chadd, Dr. P. Butler, Dr. J.M. Sykes

Acoustic microscopy, scanning Kelvin probe and AC impedance are being used to investigate factors influencing corrosion in coated tinplate and other metal containers. (In collaboration with Crown Cork and Seal Co.)

III - SURFACE REACTIONS AND CATALYSIS

Controlled atmosphere analytical electron microscopy

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

A 400 kilovolt analytical transmission electron microscope has been extensively modified and equipped with special controlled-atmosphere specimen stage. A number of projects of chemical and materials interest are now being undertaken, e.g. the study of catalysts under their working environments.

In-situ observation of solid-state reactions

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

The controlled environment TEM is being used in a study of oxidation and reduction reactions of Nb, W and Mo.

Catalytic atom probe

P. Bagot, 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, is being developed in order to permit the atomic scale study of catalytic reaction processes. (*Free University of Brussels.) (Funded by EPSRC and JIF, and in collaboration with Johnson Matthey.)

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F. Characterisation

I - SCANNING TUNNELLING AND ATOMIC FORCE MICROSCOPY

The surface structure of alternative gate dielectrics

D.T. Newell, 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 growth of $SrTiO_3$ on silicon, and silicon on $SrTiO_3$. In particular, the surface structure and composition of the $SrTiO_3$ layers will be of major importance and studied in detail by scanning tunnelling microscopy (STM) and medium energy ion scattering (MEIS). This research is sponsored by EPSRC and Oxford Applied Research.

AFM of aqueous bio-systems

C. Ramanujan, Professor A.B. Watts, Professor J.B. Pethica***

We have recently used a new AFM to resolve the solvation layers in water. The low amplitude AFM technique is now being applied to image the structure near peptides inserted at low density in lipid layers. (*Dept. of Biochemistry; **Trinity College, Dublin)

New force microscopy techniques in ambient

*C. Ramanujan, Professor J.B. Pethica**

A new, high resolution AFM which functions in liquids has been developed. We have successfully observed normal and lateral stiffness fluctuations due to individual molecular layering. The unusual shear properties of the final liquid molecular layers adjacent to a solid are being studied. (*Trinity College, Dublin)

Growth and characterization of nitride semiconductor nanostructures

Professor G.A.D. Briggs, Dr. M.R. Castell, Dr. C. Norenberg, Professor A.P. Sutton

The growth and properties of epitaxial nitride semiconductor nanostructures are studied, with a view to discovering materials systems that may be useful for quantum structures. Islands are grown in our variable temperature STM, and examined in situ. We investigate factors that affect their shape and size distributions, the phases that are present, and the surface structures and electronic properties. Atomistic and multiscale modelling enables the structure of surfaces and interfaces to be elucidated, and the distribution of island types and sizes to be accounted for. (Funded by The Royal Society)

Nanostructures on the SrTiO3 (001) Surface

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

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

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)

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

Dr. C. Norenberg, 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. (*TU-Ilmenau, Germany) (In collaboration with Hewlett-Packard Laboratories) (Funded by EPSRC and The Royal Society)

Growth and spectroscopy of metallic nanoislands

Dr. F. Silly, A.C. Powell, 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)

II - FIELD-ION MICROSCOPY AND ATOM PROBE MICROANALYSIS

Atom probe microanalysis techniques

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

The combination of field-ion microscope and atom probe techniques allow us to image the surface of materials with atomic resolution and perform microanalysis of sub-nanometre regions or layers within the specimen. We are continuing the development of the Position Sensitive Atom Probe (PoSAP), which can provide a full 3-dimensional reconstruction of atomic-scale composition variations in materials. The latest generation of this instrument includes an optically coupled multi-hit detector system, and uses a reflectron lens to increase mass resolution to $m/\Delta m=600$ full-width at half maximum. A new instrument is currently being built to extend the technique to the study of catalysis. (Funded by EPSRC and JIF and in collaboration with Oxford Nanoscience Ltd. and Johnson Matthey plc.)

Early stages of precipitation in 7xxx series aluminium alloys

*Dr. J.C. Oh, Professor A. Cerezo, Dr. A. Alam**

A combination of 3-dimensional atom probe and positron annihilation spectroscopy is being used to characterise the early stages of precipitation in 7xxx series Al alloys. The objective of this study is to provide thermodynamic and kinetic parameters which will allow computer simulation of the precipitation process. (*Bristol University) (In collaboration with Alcoa.)

Scanning atom probe

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

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

Atom probe analysis of information storage materials

S.H. Lee, S. Pinitsoontorn, Professor A. Cerezo, Professor A.K. Petford-Long, Dr. P. Clifton, Dr. D.J. Larson**

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. (*Seagate Technology) (Funded by EPSRC and Seagate Technology)

3D Reconstruction of atom probe data

Dr. G. Chapman, Dr. P.J. Warren, 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.)

Atom probe studies of 2xxx Al alloys

L. Davin, Professor A. Cerezo

A study is being performed of the precipitation in new damage tolerant 2xxx series aluminium alloys. The 3-dimensional atom probe is being used to characterise the composition and morphology of nanometre sized phases and the partitioning of alloying elements. (Project in collaboration with the University of Southampton and Imperial College.) (Funded by EPSRC, Airbus and QinetiQ)

Early stages of precipitation in 6XXX automotive sheet

A. Morley, D. Vaumousse, Professor A. Cerezo

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. (In collaboration with Alcan International)

Thermal ageing of steels

Dr. G. Sha, 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.)

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

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

High resolution electron microscopy (HREM)

The Department's 400 kilovolt JEOL 4000EX(II) electron microscope has a point-to-point resolution of 0.16nm with an information limit approaching 0.12nm; this is currently better than any other conventional TEM 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 a CCD camera and an on-line TV system.

Analytical electron microscopy (AEM)

A Philips CM20, a routine 200 kV AEM with full analytical facilities. 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).

High resolution analytical electron microscopy

A JEOL 2010 high resolution electron microscope combines high spatial resolution (down to 0.19 nm) with a two nanometre diameter electron probe for nano-diffraction or convergent beam diffraction. An energy-dispersive X-ray analysis capability and an on-line TV imaging system make this a very versatile instrument. It is being used in a wide range of projects, with particular emphasis on microstructural characterization of nanocomposites.

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.

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), 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 transmission electron microscopy (STEM)

The VG HB501 STEM has a high brightness field emission gun (FEG) and facilities for microanalysis from selected areas of 1nm in diameter. Microanalysis techniques include energy dispersive x-ray spectroscopy (EDS) and electron energy loss spectrometry (EELS). The beam size and stability gives sub-monolayer sensitivity for grain boundary segregation analyses. External computer control has been implemented for a flexible approach to mapping and linescan techniques. The gun and specimen chambers are all ultra-high vacuum ($<1x10^{-10}$mbar). The instrument is used primarily for combined structural and chemical analyses of interfaces.

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 LaB6 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 and is presently undertaking acceptance tests. 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 an FEI FIB2000 TEM system that will be 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.

Development of an aberration-corrected electron microscope for high resolution analysis and imaging

Professor D.J.H. Cockayne, Professor J.M. Titchmarsh, Dr. J.L. Hutchison, Dr. A.I. Kirkland, 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 will provide analysis and spatial resolution capabilities a the 1 Å level. The instrument will be used for atomic-scale investigations of a range of new materials. (Funded by JIF)

Nanoscale Dynamic Chemistry using Environmental Transmission Electron Microscopy

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

This project aims to provide examine a wide range of materials in the TEM under accurately controlled gas atmospheres at elevated temperatures and variable pressure. These will be studied in situ and in real time and the data will be acquired digitally. In this way we hope to provide new insights into the thermodynamics and kinetics of solid state processes on the nanoscale. We also plan to investigate the in-situ formation of several families of nanostructures. In parallel it may be possible to develop the theoretical and computational tools necessary to understand the nature of the complex electron beam gas interactions the results of which will be used to quantify the experimental images obtained. (Funded by EPSRC)

Nanometer scale induced structure between amorphous layers and crystalline materials

Professor D.J.H. Cockayne, Professor A.P. Sutton, Dr. C. Marsh, Dr. M. Doblinger, Dr. C.M. Bishop+, Professor M. Ruhle, Professor M. Hoffmann**, Dr. M. Gautier-Soyer***, Professor C. Carter +, Professor Y-M. Chiang, Professor R. French, Professor Garofalini +++, Professor W-Y. Ching, Dr. R. Cannon*

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, University of Missouri-Kansas; and Lawrence Berkeley Lab, San Francisco.

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. (Funded by The Royal Society)

Electron back scatter diffraction

Dr. A.J. Wilkinson

Electron back scatter diffraction patterns are used to measure the orientations of individual grains and grain boundary misorientations in polycrystals. The method is being applied to characterise crystallographic textures in a variety of materials systems: Al-Li alloys, Ni-based superalloys, steels, metal-ceramic interfaces, and superconductors. New analysis methods are being developed for the measurement of small angle misorientations developed during plastic deformation and for the measurement of local elastic strain tensors. (Funded by The Royal Society)

Disorder in complex oxides

Dr. J.L. Hutchison, 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. (Funded by British Council)

The structure of copper precipitates in age-hardening steels

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

High-resolution and analytical transmission electron microscopy is being used to study the structure and chemistry of Cu-rich precipitates in age-hardening martensitic and maraging stainless steels, which appear similar to those found in irradiated pressure-vessel steels and model alloys. The potential of energy-selected imaging (using the Gatan imaging filter on the Jeol 3000F FEGTEM) is being explored. (Funded by EPSRC)

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) (Funded by UK-Israel Research Fund)

Electron probe microanalysis of multicomponent materials

Dr. M.L. Jenkins, C.J. Salter, Dr. C.R.M. Grovenor, Dr. J.T. Czernuszka, Dr. P.S. Grant, Dr. E. Young, Dr. E. McClelland*, Professor R.K. O'Nions**

A state of the art electron-probe X-ray analyser (JEOL JXA 8800RL) has been installed for composition analysis and mapping of a wide variety of complex multicomponent metals, ceramics, composites, biomaterials and minerals.(*Department of Earth Sciences) (Funded by JREI)

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, Dr. M. Doeblinger, Dr. D. Nguyen Manh**

Techniques for investigating the structure of amorphous thin films and small volumes of amorphous materials are being developed using energy selected electron diffraction combined with atomistic modelling. Refinement procedures are being developed which will allow differentiation between alternative structural models. (*UKAEA, Culham) (Funded by EU and JEOL)

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

Dr. A.I. Kirkland, Dr. J.L. Hutchison, Dr. J. Sloan, Dr. R.R. Meyer

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. (Funded by EPSRC, Leverhulme Trust and The Royal Society)

Quantum dot segregation

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

The geometry and composition of quantum dots in semiconductor materials is being investigated with a range of electron optical techniques including HREM, energy filtered EM, and image simulations. Atomistic modelling combined with monte Carlo techniques is being used to investigate models of segregation. (*UKAEA)

3-D microstructural analysis using a FIB system

Dr. R.M. Langford, Professor J.M. Titchmarsh, Dr. B.J. Inkson, Dr. G. Mšbus**

A focused ion-beam system is being used to mill 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)

Fabrication of site-specific 3-dimensional atom-probe specimens

Professor A.K. Petford-Long, Professor A. Cerezo, Dr. P. Clifton, Dr. D.J. Larson**

The FIB is being used to develop methods to prepare site-specific 3-dimensional atom-probe specimens from flat samples such as magnetic multilayer films, so that the magnetic and transport properties can be directly compared with the 3-dimensional morphology. (*Seagate Technology) (Funded by EPSRC and Seagate Technology)

Development of an advanced FIB system for micromachining applications

Dr. R.M. Langford, Professor A.K. Petford-Long

Novel techniques based on the use of a focused ion-beam system are being developed. These are primarily aimed at micromachining of a range of materials systems such as magnetic devices, optoelectronic devices and embossing heads. The aim is to develop techniques for the fabrication of structures with high depth:width aspect ratio and curved side-walls. (Funded by EPSRC)

Investigation of carbon nanotubes produced by novel synthetic methods

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

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)

NanoSIMS analysis of Biological Materials

K. Smart, A. Green, Dr. M. Kilburn, Dr. C.R.M. Grovenor, Dr. J.T. Czernuszka, Professor J. Dilworth, Professor J.A.C. Smith***

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 will be dedicated to studies of biological materials. Current projects include

[1] the analysis of the mechanisms for heavy metal transport and accumulation in hyperaccumulator plants

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

[3] Trace element localisation in human teeth and bone samples (in collaboration with Proctor and Gamble, University of Manchester and Shire Pharmaceuticals).

(* Department of Chemistry, **Department of Plant Sciences) (Funded by EPSRC JIF)

NanoSIMS analysis of metallic and electronic materials

C. Dark, S. Ahmed, S. Haigh, Dr. C.R.M. Grovenor, Dr. M. Kilburn, 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] Analysis of the distribution of H in aluminium castings (in collaboration with Dr K O'Reilly)

[3] The chemistry of trace elements in structural steels (in collaboration with Corus)

[4] Impurity and light element analysis in MgB_2 wires and powders

Development of FIB machining

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)

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)

New Detectors for Transmission Electron Microscopy

Dr. A.I. Kirkland, Dr. R.R. Meyer

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)

Structure of Interfaces between crystalline and amorphous materials

Professor D.J.H. Cockayne, Dr. M. Doeblinger, M. Bruin

HREM is being used to investigate the structure of interfaces between amorphous and crystalline regions of intergranular films in ceramics. The aim is to determine the crystallographic orientation and the extent of planarity of these interfaces. (Funded by EU)

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, Professor G.D.W. Smith, Dr. M Dovey*, Dr. A.I. Kirkland, Dr. R.R. Meyer*

Remote access to electron microscopes is being developed. The aim is to develop a capability of persistent and pervasive access, using the e-Grid. A dedicated SEM has been installed, and remote access is being "rolled out". over time. (Funded by DTi and Jeol)

Electron Energy Loss studies of nanostructures

Professor D.J.H. Cockayne, Dr. D.A. Pankhurst, 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)

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. (*Seagate Technology) (Funded by EPSRC and Seagate Technology)

Gram quantities of pure carbon nanotubes and related materials

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.

Aberration-corrected high resolution electron microscopy

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

We are exploring ways of exploiting the facility to adjust 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. (Funded by EPSRC JIF)

Novel Approaches to Direct Object Reconstruction in Transmission Electron Microscopy

Dr. A.I. Kirkland, Dr. R.R. Meyer

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 experiments capable of achieving sub Angstrom resolution and may be applicable to imaging and diffraction using other radiation sources. (Funded by EPSRC)

IV - RADIATION DAMAGE

Contributions of Inelastically Scattered Electrons to Defect Images and Diffraction Patterns.

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

The availability within the department of the JEOL 3000F FEGTEM equipped with a Gatan Imaging Filter (GIF) and CCD camera has opened up new opportunities for exploring more systematically the advantages of energy-filtered imaging and diffraction, and determining more precisely the contributions to images and diffraction patterns of inelastically scattered electrons. 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 diffraction pattern simulations. (*Argonne National Laboratory) (Funded by US Department of Energy via ANL, EURATOM/UKAEA)

Quantum Electron Microscope Imaging of Nanoclusters under Weak-Beam Conditions

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

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 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. (*EURATOM/UKAEA ** Argonne National Laboratory) (Funded by EURATOM/UKAEA)

Transmission electron microscopy of fusion neutron cascades

Dr. M.L. Jenkins, C. Creighton

The first wall of future fusion reactors will be bombarded with high fluxes of very energetic (14 MeV) neutrons produced in the fusion reaction. These neutrons will create radiation damage in the form of ‘displacement cascades’ - branching series of collisions between displaced ‘knock-on’ atoms, producing thousands of Frenkel pairs in a volume of typical dimensions a few tens of nanometers. The theory group of Prof. Sutton has recently started modelling of very energetic cascades. This project will complement the modelling studies by studying experimentally fusion-neutron cascades in the ordered alloy Cu_3Au, which can be imaged directly in the TEM via local regions of reduced long-range order (‘disordered zones’) which are produced at cascade sites. Small point-defect clusters produced by radiation damage of materials relevant to fusion reactors will also be studied.

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 the precipitation of copper-rich particles, and the identification of the matrix component of hardening. (Funded by EPSRC)

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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 and Silicon Graphics 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.

Experimental-theoretical study of alloying behaviour of high-temperature transition metal silicides

Professor D.G. Pettifor, Dr. D. Nguyen Manh, Dr. D.A. Pankhurst, Professor P. Tsakiropoulos**, Professor V. Vitek****

The X-ray spectra, phase stability and bonding behaviour of molybdenum disilicide alloyed with chromium and aluminium are being studied both theoretically (in Oxford) and experimentally (in Surrey). (*UKAEA, Culham; **University of Surrey; ***University of Pennsylvania) (Funded by EPSRC)

MBE growth of spintronic materials

Professor D.G. Pettifor, Dr. R. Drautz, D. Murdick, 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).

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)

Power dissipation in metallic nanowires

*Professor A.P. Sutton, Dr. T.N. Todorov**

The purpose of this project is to implement a tight binding formalism to simulate power dissipation and local heating in current-carrying nanowires, and to combine the heating simulations with existing tight binding calculations of current-induced forces. (*Queen's University Belfast) (Funded by EPSRC)

Dynamical Ising model simulations of phase separation

Dr. G. Sha, Dr. A. Schneider, 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). (*AEA Technology, Harwell) (Funded by Rolls Royce)

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. (Funded by Hewlett-Packard Labs.)

Modelling short fatigue crack growth through polycrystals

Dr. A.J. Wilkinson

Models are being developed for short fatigue crack growth based on dislocation mechanics descriptions of crack - plastic zone - grain boundary interactions. The effects of grain size, grain orientation, and grain boundary misorientation distributions are being incorporated through a Monte-Carlo scheme allowing the microstructure induced statistical variations in short fatigue crack growth behaviour to be analysed.

Current-induced effects in molecules

Professor A.P. Sutton, M. Todorovic

Current-induced mechanical and heating effects in molecular systems are being modelled.

Modelling adhesion between polymers and inorganic substrates

*Professor A.P. Sutton, Dr. D.R. Mason, Dr. T.R. Walsh**

A new strategy for modelling adhesion between polymers and inorganic substrates has been developed. It is being applied to polymer adhesion issues of interest to the semiconductor industry. This project is part of an e-science collaboration called 'RealityGrid', funded by EPSRC. (*Warwick University) (In collaboration with Loughborough and Manchester computing centres and UCL)

Carbon-based nanostructures

Professor E.G. Wang, Professor Lianmao Peng*, Dr. Bang-gui Lui*, Dr. D. Nguyen Manh**, Professor D.G. Pettifor*

The structure, of carbon-based nanostructures is being predicted using semi-empirical Tight Binding and first principles Density Functional Theory, and being compared with electron microscope images. (*Centre for Condensed Matter Physics, Beijing, China; **UKAEA, Culham) (Funded by Royal Society -CAS joint research project)

First principle studies of intermetallics

H.R. Chauke, M. Phasha*, Professor P.E. Ngoepe*, 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)

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

*K. Kawata, Dr. V.M. Burlakov, Dr. M. Carey, Professor A.P. Sutton, 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)

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.

Modelling the structure of amorphous oxide films grown by vapour deposition

Professor A.P. Sutton, Dr. V. Burlakov, S. van Alfthan, Professor K. Kaski**

A new Monte Carlo technique has been developed and applied to the growth of SiOx films by vapour deposition. The technique enables the structures of network forming oxide films to be modelled, and provides information about radial and bond angle distribution functions as well as porosity. The technique is now being extended to other amorphous oxides and amorphous elements grown by vapour deposition. (* Helsinki University of Technology)

Modelling the evolution of cascades in fusion reactor materials

*Professor A.P. Sutton, T.S. Hudson, Dr. S.L. Dudarev**

Fusion reactor materials are subjected to neutron irradiation with energies in excess of 14MeV. These neutrons produce cascades of damage which evolve over time into defects and defect clusters. The temporal evolution of the cascade damage will be modelled by Monte Carlo simulations, with particular attention to long-range elastic interactions. (*UKAEA Fusion, Culham Science Centre) (Funded by UKAEA Fusion)

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)

Unresolved issues in giant magnetoresistance

Professor D.G. Pettifor, Professor E. Yu. Tsymbal, Dr. R.J. Baxter, Professor B. Hickey**, Dr. S. Thompson****

Unresolved issues in magnetoresistance and current-in-plane (CPP) giant magnetoresistance (gmr) are being investigated using a tight-binding model of conduction. There is collaboration with the experimental groups at York and Leeds. (*University of Nebraska at Lincoln, **University of Leeds, ***University of York) (Funded by EPSRC)

Modelling carbon nanostructures for quantum computing

Dr. S.M. Lee, R. Scipioni, D. Gunlycke, Dr. D. Nguyen Manh, 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. (*UKAEA, Culham). (Funded by EPSRC Foresight LINK Project, DTI and Hitachi Europe).

Simulations of TEM abberation corrected images

Professor J.M. Titchmarsh, L.Y. Chang, Dr. A.I. Kirkland

This project will provide image simulations under conditions now achievable in the recently installed double Cs aberration corrected TEM in the Department.

Brittle-Ductile Transitions in Silicon

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

Recent experiments in David PopeÕs group show that single crystal beams of silicon, initially free of dislocations, yield abruptly at a strain-rate dependent critical stress when loaded in 3-point bending at elevated temperatures. A model is being developed, supported by computer simulation, to explain these results in terms of the generation of dislocations at a knife edge, and their motion from the compressed to the tensile surface of the beam, followed by specific cross-slip events to form dislocation sources.

Quantitative Atomic resolution Imaging

Dr. 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.

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).

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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 and precious metallurgy in the European Iron Age

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

The study of copper-based and precious metal alloys from excavations and hoards of the pre-Roman Iron Age is leading for the first time to an understanding how these metals were made and traded in a period when iron had become the dominant utilitarian metal. Material is now available to illustrate how production on individual sites was organised and what techniques were used together. Attention is also focused on cemeteries to look for associations between gender and status of individuals and the technical quality of artefacts buried with them. (*Abteilung Ur-und Frühgeschichte, Universitüt Zürich, Switzerland; **Institut für Ur-und Frühgeschichte, Universität Wien, Austria)

Application of microprobe and metallographic techniques to numismatic problems

Dr. J.P. Northover, Dr. D.M. Metcalf, Dr. C.E. King*, Dr. L. Treadwell**

The Cameca SEMPROBE is used to study the copper-, silver- and gold-based alloys used for a variety of coinages. Current projects involve Roman base-silver coinages of the later 3rd century AD, the silver and base-metal coinages of medieval England, the coinage of the pre-Roman Iron Age, Indo-Greek and Islamic coinages. Very large databases of analyses have been and are being assembled in all these areas and attention is now directed to new methods for interrogating these. (*Ashmolean Museum, Oxford)

Early metallurgy in the Upper Euphrates Basin

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

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 B.C. during the period in which 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 focused our attention on the great importance of recycling in these early cities. (*University of Manchester; **Department of Archaeology, University of Durham).

The use of high resolution scanning Auger microscopy to characterise internal corrosion in archaeological bronze

Dr. J.P. Northover, Dr. E. Paparazzo*, Dr. D. Baer**, Dr. S. Lea***

The mechanisms of long-term corrosion processes of buried bronze surfaces are beginning to be well understood. Much less clear are those involved in sub-surface and internal inter- and transgranular corrosion in the same objects. The approach used here is to maximise the resolution obtainable with scanning Auger microscopy in mapping corrosion species at grain boundaries in bulk samples. Resolutions of the order of 10nm have been obtained in elemental mapping; the interpretation of these maps is now being developed. (*ISM-CNR, Frascati, Roma, Italy; **Pacific Northwest National Laboratory, Richland, WA, USA)

Investigation of the relationship between slag inclusion compositions and welding practice

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

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

Effects of cremation on copper alloys

Dr. J.P. Northover

The effects of high temperatures on copper alloys in oxidising, neutral and reducing atmospheres is being studied by optical metallography and by experimental replication. The results are used to determine the placement of grave goods in cremation pyres to assist in interpreting the burial rites. (In collaboration with Wessex Archaeology)

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

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

The requirements of museum collections have stimulated this project in non-destructive and minimally destructive analysis of ancient bronze. The aim is to use a laser to mill sub-millimetre diameter windows in the patina on selected bronzes and then use the SPM to analyse the metal as it is exposed, with the X-ray mapping facility employed to make basic metallographic observations. An experimental programme will develop the best mode of operation and assess the quality of the analyses in comparison with sample-based analysis. (*University of Surrey)

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

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

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

Copper extraction at Ross Island, Co. Kerry, Ireland

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

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

The characterisation of Islamic steels

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

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

The development of iron and steel for structural and railway use in the 19th century.

Dr. J.P. Northover

Rails and structural iron and steelwork surviving from the nineteenth century are often well dated and provenanced to specific ironworks. They offer an ideal means of studying developments in the capabilities of, successively bloomery iron, puddled iron and Bessemer steel for such products. A successful pilot project has led to new connections so that, for instance, it will be possible to compare practice in Britain and France

A study of Byzantine copper alloy metalwork

*Dr. J.P. Northover, Dr. M. Saghieh Beydoun**

An analytical and metallographic study of early Byzantine copper alloy metalwork based on the excavations in Beirut. The site was sealed by an earthquake in 551 AD so this study enables us to characterise everyday Byzantine metalwork at a particular moment in time. (*Lebanese University, Beirut) (Funded by British Council)

Metalwork of the Bronze Age-Iron Age transition in Britain

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

Combining archaeological and metallurgical methods to understand metalwork and metalworking in Britain at the time of the first introduction of iron in the 8th-6th centuries BC. This is the first ever systematic survey of this material. (*Institute of Archaeology, University of Oxford)

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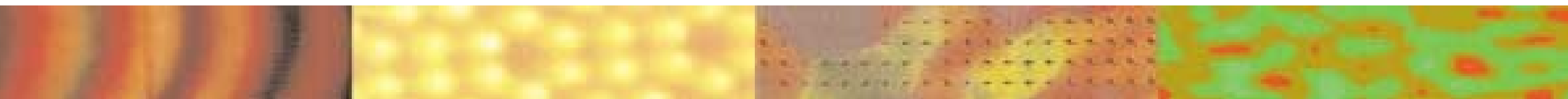

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