



Research in Progress
2001 - 2002



Department of Materials

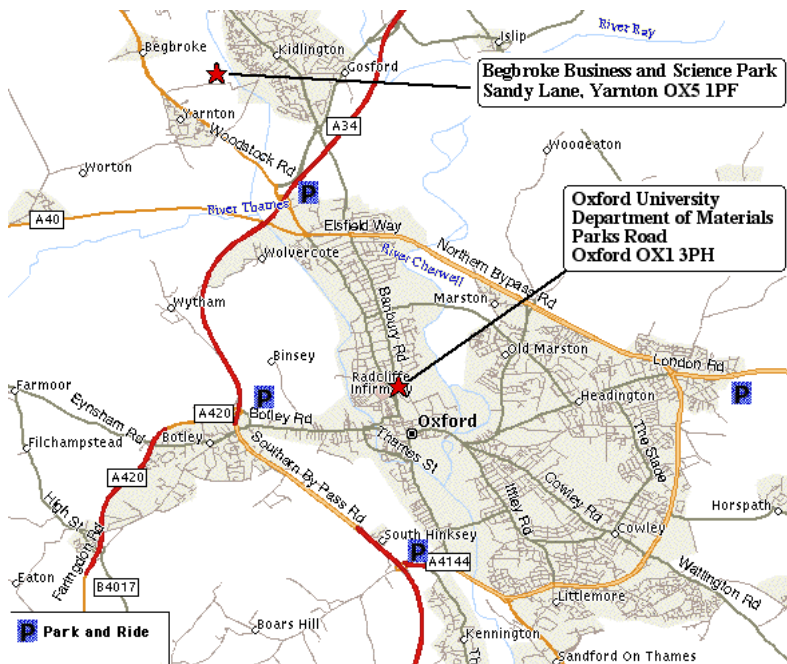


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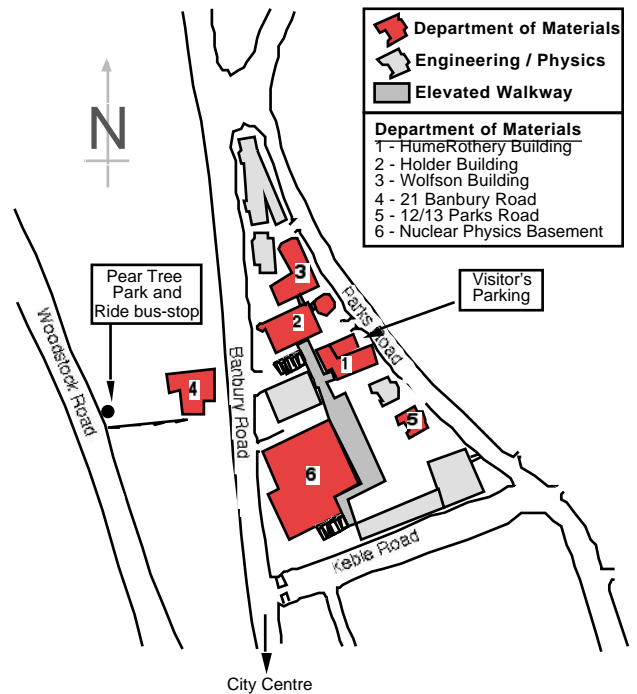
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Department of Materials

University of Oxford

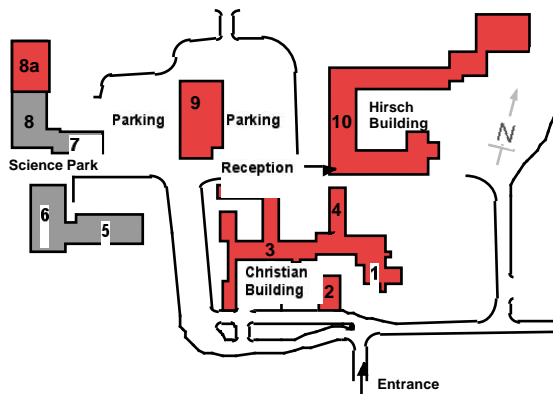


Department of Materials Keble Road Triangle



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| <p>Department of Materials & OCAMAC</p> <ul style="list-style-type: none"> 10 Hirsch Building - Reception - Infineum Laboratories - AEA Laboratories - Materials Laboratories - Luxfer ATC - JEOL Laboratories <p>3 Christian Building</p> <ul style="list-style-type: none"> - Offices - Infineum Offices - AEA Clean Room <p>1 Manor House</p> <p>4 Conference Suite</p> <p>9 Storage Barn</p> <p>Business & Science Park</p> <ul style="list-style-type: none"> 2 Yarnton Security Services 5 Innovation Centre 6 Prolysis 7 Nanox 8 Opsys |
|--|

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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 top gradings for both teaching and research in the government's most recent assessment exercises, and we continue to make outstanding progress in the pursuit of our objectives. Major advances over the last four years include:

- 1 Three new Professorships, in electron microscopy (David Cockayne), structural integrity (John Titchmarsh) and nanomaterials (to be appointed);
- 2 Three elections to Fellowships of the Royal Society (David Cockayne, John Pethica and John Hunt) 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 (John Pethica), the Institute of Materials Platinum Medal (John Martin), 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 (Sir Peter Hirsch).
- 4 Two promotions to personal professorships (Adrian Sutton and Andrew Briggs) and eight promotions to readerships (Alfred Cerezo, Patrick Grant, Chris Grovenor, John Hutchison, Mike Jenkins, Amanda Petford-Long, Steve Roberts, 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 award of a major 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 about 30 academics, 50 senior researchers, 35 technicians and secretaries, 60 postdoctoral researchers, 20 visitors, 75 research students and 120 undergraduates. The Department is part of an integrated Division of Mathematical and Physical Sciences at Oxford, which includes physics, chemistry 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.

Oxford
October 2001

Professor G.D.W. Smith FRS
Head of Department

Member of Department

Professors

Professor G.D.W. Smith, FRS	<i>Head of Department</i>
Professor B. Cantor, FREng	<i>Cookson Professor of Materials Head of Division of Mathematical and Physical Sciences</i>
Professor D.J.H. Cockayne, FRS	<i>Professor in Physical Examination of Materials</i>
Professor D.G. Pettifor, FRS	<i>Isaac Wolfson Professor of Metallurgy</i>
Professor J.M. Titchmarsh	<i>The Royal Academy of Engineering/AEAT / INSS Research Professor in Microanalysis and Structural Integrity</i>
Professor G.A.D. Briggs	<i>Professor of Materials</i>
Professor R.J. Brook, OBE FREng	<i>Professor of Materials</i>
Professor B.L. Eyre, FRS FREng	<i>Visiting Professor</i>
Professor Sir Peter Hirsch, FRS	<i>Emeritus Professor</i>
Professor J.D. Hunt FRS	<i>Professor of Physical Metallurgy</i>
Professor C.J. Peel	<i>Visiting Professor</i>
Professor J.B. Pethica, FRS	<i>Visiting Professor</i>
Professor A.P. Sutton	<i>Professor of Materials Science Director of the Materials Modelling Laboratory</i>
Professor M.J. Whelan, FRS	<i>Emeritus Professor</i>
Professor J.V. Wood	<i>Visiting Professor</i>

Readers

Dr. C.R.M. Grovenor	<i>Deputy Head of Department</i>
Dr. A. Cerezo	<i>Director of Graduate Studies</i>
Dr. P.S. Grant	<i>Director of Oxford Centre for Advanced Materials and Composites Director of Faraday Partnership in Aerospace and Automotive Materials</i>
Dr. M.L. Jenkins	<i>Director of Electron Microscopy Facilities</i>
Dr. J.L. Hutchison	<i>Reader in Materials</i>
Dr A.K. Petford-Long	<i>Reader in Materials</i>
Dr. S.G. Roberts	<i>Reader in Materials</i>
Dr. J.M. Sykes	<i>Reader in Materials</i>

Lecturers

Dr. H.E. Assender	<i>Lecturer in Materials</i>
Dr. D.G. Bucknall	<i>Lecturer in Materials</i>
Dr. J.T. Czernuszka	<i>Lecturer in Materials</i>
Dr. G.W. Grime	<i>Lecturer in Materials</i>
Dr. P.J. Northover	<i>Lecturer in Materials</i>
Dr. K.A.Q. O'Reilly	<i>Lecturer in Materials</i>
Dr. R.I. Todd	<i>Lecturer in Materials</i>
Dr. P.R. Wilshaw	<i>Lecturer in Materials</i>

Administration

Dr. R.M. Plummer	<i>Administrator</i>
Mrs. D. Faulkner	<i>Deputy Administrator</i>
Ms. M. McClung	<i>Deputy Administrator</i>

Senior Research Fellows

Dr. R. Ball	Wolfson Industrial Fellow	Dr. O.V. Kolosov	EPSRC Advanced Fellow
Dr. S. Benjamin	Royal Society Research Fellow	Dr. J.W. Martin	OCAMAC Senior Fellow
Dr. G.R. Booker	OCAMAC Senior Fellow	Dr. G. Möbus	EPSRC Advanced Fellow
Dr. M.R. Castell	Royal Society Research Fellow	Dr. C. Nörenberg	RS Dorothy Hodgekin Fellow
Dr. J. Coyle	OCAMAC Senior Fellow	Dr. O.V. Salata	OCAMAC Industrial Fellow
Dr. A. Crossley	Senior Visiting Fellow (AEAT)	Dr C. Sofield	Senior Visiting Fellow (AEAT)
Dr. A. Daykin	Senior Visiting Fellow (QinetiQ)	Dr. P. Schumacher	EPSRC Advanced Fellow
Dr. R. Falster	OCAMAC Senior Fellow	Dr. C.B. Scruby	Wolfson Industrial Fellow
Dr. B. Gilmore	Senior Visiting Fellow	Dr. J. Sloan	Royal Society Research Fellow
Dr. R. Harper	Senior Visiting Fellow (AEAT)	Dr. I.C. Stone	Senior Research Fellow
Prof. R. Howson	Senior Visiting Fellow	Dr. G. Taylor	Senior Research Fellow
Dr. D. Imeson	Senior Visiting Fellow (DSDL)	Dr. D. Vesely	OCAMAC Senior Fellow
Dr. B.J. Inkson	Royal Society Research Fellow	Dr. T.R. Walsh	Glasstone Research Fellow
Dr. C. Johnston	Senior Research Fellow (AEAT)	Dr. A.J. Wilkinson	Royal Society Research Fellow

Research Fellows

Dr. K.H. Baik	Dr. J-H. Kang	Dr. H. Peng
Dr. M.S. Bobji	Dr. K.R. Kirov	Dr. K. Porfyraakis
Dr. V. Burlakov	Dr. R. Langford	Dr. F. Prima
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Mr. R.C. Doole	Dr. R. Matthews	Dr. E. Tsymbal
Mr. T.J. Godfrey	Dr. W. McBride	Dr. Y-G. Wang
Dr. C. Gras	Dr. M. Moniruzzaman	Dr. B. Warot
Dr. R. Hansen	Dr. Duc Nguyen Manh	Dr. P.J. Warren
Dr. B.M. Henry	Dr. H. Nörenberg	Dr. D. Whittle
Dr. C.J.D. Hetherington	Dr. I. Oleinik	Dr. H. Wu
Dr. S. Hirosawa	Dr. I.G. Palmer	Dr. M. Yun
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Dr. Y. Huang	Mrs S. Panteny	

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Mr. A. Gould	Mrs. L. Richmond	Mr. L. Walton

D.Phil and MSc. Research Students

Abraham, M. (EPSRC)	Leigh, D. (EPSRC Foresight Link)
Abraham, M.H. (self-supporting)	Lozano-Perez, S. (EPSRC / St Annes Scholarship)
Allsop, N. (EPSRC / St. Annes Scholarship)	Manson-Whitton, C.D.J. (Royal Commission for the Exhibition of 1851 Scholarship / Luxfer Ltd.)
Austwick, M.R. (EPSRC)	Mason, D. (EPSRC / Applied Materials Linacre Scholar)
Bagot, P. (EPSRC)	Mathieson, D.
Barnes, J-P. (EPSRC)	Morgan, D.L. (EPSRC)
Bernardo, C. (self-supporting)	Morley, G. (EPSRC Foresight Link)
Boon, P.M. (EPSRC)	Nazir, A. (EPSRC)
Briceno-Gomez, M. (Qinetiq)	Okayasu, T. (Oji Paper Co.)
Brown, G. (CASE: Colebrand Ltd.)	Oliver, R.A. (EPSRC)
Burman, T. (CASE: Regenesys)	Ortiz-Merino, J.L. (Mexican Government)
Campbell, P.J.D. (CASE: BNFL)	Owen, N.W. (EPSRC)
Carter, R. (EPSRC)	Pak, S.J. (Self-supporting)
Castro Diaz, L. (Regenesys / Linacre)	Park, S-B. (self-supporting)
Chandrapalan, P. (CASE: Regenesys)	Pongsaanutin, T. (Thai Government)
Chilton, A. (CASE: Alcan)	Ramanujan, C.S.
Choi, Y-S. (EPSRC)	Rayment, T. (EPSRC / St. Cross Scholarship)
Coates, M. (EPSRC)	Ruitenbergh, G. (EPSRC)
Cockfield, T. (CASE: Alcan)	Russell-Stevens, M.J. (EPSRC)
Davidson, I. (CASE: Alcoa Extrusions)	Sachlos, E. (St. Peter's College)
Davin, L. (EPSRC)	Saunders, S. (CASE: National Physical Laboratory)
DeArdo, I. (self-supporting)	Scipioni, R. (Self / EPSRC Foresight Link)
DeMorais, A. (Nordiko Ltd)	Shin, M. (CASE: Alcan)
Di Maio, D. (Hardide)	Simmons, P. (CASE: T&N Technology)
Doherty, M.J. (EPSRC)	Speller, S. (EPSRC)
Erlat, A.G. (Toppan)	Srimanosaowapak, S. (Thai Gov.)
Galano, M. (EU/Korea/Clarendon/ORS)	Steer, T. (EPSRC)
Giannattasio, A. (MEMC Ltd.)	Stowe, D.J. (EPSRC)
Gilberti, L. (EPSRC)	Taylor, R.N. (CASE: Nanox)
Gledhill, S. (EU)	Trancik, J. (Rhodes Scholarship)
Gomez-Morilla, I. (BNSC)	Tzvetkov, B. (Scatcherd / ORS)
Gotora, D. (Rhodes)	Vaumousse, D. (CASE: Alcan International Ltd.)
Gunlycke, D. (EPSRC Foresight Link)	Wain, N. (EPSRC)
Hedges, M.K. (EPSRC)	Whiteley, R.M. (EPSRC)
Hudson, T. (AEA / Linacre)	Whyte, E. (CASE: Corus)
Jiansirisomboon, S. (Thai Government)	Wilkinson, S. (EPSRC / Guy Newton Wolfson Scholar)
Kim, H.S. (self-supporting)	Wu, H. (Research Assistant)
Kim, K-B. (self-supporting)	Xu, J. (self-supporting)
King, O. (EPSRC)	Yoo, K-D. (British Council/Hyundai Electronics, Korea)
Kurum, E. (EPSRC)	Zhang, L. (ORS)
Lambourne, A. (Department)	Zhou, Z. (UKAEA)
Langham, C. (Motorola)	Zhu, M. (K.C.Wong / ORS)
Lang, C. (EPSRC)	

Part II Students

Metallurgy & Science of Materials

Beer, N.L.

Booth, S.

Bromwich, T.J.

Buckley, J.

Cornick, A.O.

Dark, C.J.

Eggeman, A.

Gourlay, C.

Kathuria, R.

Martin, S.P.

Perry, T.O.R.

Shapiro, I.

Walpole, A.R.

Ward, C.

Waring, M.

Wearden, A.M.

Engineering and

Materials Science

Birkinshaw, M.A.

Grigorov, A.V.

Lynesmith, D.L.

Winch, M.F.D.

Materials, Economics and Management

Bradbury, A.R.

Ivell, T.

Kim, K-J.

Leary, E.W.

Palmer, R.

Wilkinson, E.K.

Visiting Academics

Dr. F.E. Audebert, University of Buenos Aires, Argentina

Prof. V.V. Baranauskas, Campinas State University, Brazil

Dr. R. Bhatti, QinetiQ

Dr. M.J. Daniels, Ann Arbor, USA

Dr A.J. Doyle, Doyle & Tratt Products Ltd

Dr. J. Du, University of Science & Technology of China

Prof. M.W. Finnis, Queen's University, Belfast

Dr. B.D. Huey, British Marshall Sherfield Fellow

Dr. R. Iqbal, Microsharp Corporation Ltd, UK

Dr S.H. Kim, Yonsei University, Seoul, S Korea

Prof. H.S. Kim, Chungnam National University, S Korea

Dr. M. Martín-Fernández, Fulbright Fellowship, Spain

Dr. M. Matsukawa, Doshisha University, Kyoto, Japan

Dr. S. Mukhopadhyay, IUCDAEF, Indore, India

Dr. N. Mustapha, University of Surrey

Prof. A.H.W. Ngan, University of Hong Kong

Prof. H. Ohsawa, Tokyo University, Japan

Dr. H.Ö. Özer, Trinity College Dublin

Dr. D. Ozkaya

Dr. A. Safonov, Opsys, Begbroke

Dr. A.J. Tolley, IAIE (Vienna) Researcher, Argentina

Dr. M. Ushirozawa, Japan Broadcasting Corporation

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Mr. A. Geddes, Metal Agencies Ltd / Viohalco Group Greece

Mr. N.P. Gregory, Abingdon School

Mrs. E. Finch, Pricewaterhouse Coopers

Mr. D.K. McLachlan, Pricewaterhouse Coopers

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Mr. C. Purcell

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.

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Luxfer Group Ltd	

Profiles of Academic Staff



Dr. Hazel Assender
Linacre College

Lecturer in Materials

Research, both experimental and modelling, on a range of polymer and polymer composite materials. Particular areas of interest include crystallinity and morphology, hydration of polymers, the relationship between processing and microstructure and surface and interface characterisation, modification and coatings. Modelling spans a wide range from atomistic modelling of crystal structure through mesoscale microstructural modelling and finite element continuum level simulations.



Dr. Simon Benjamin
Exeter College

Royal Society University Research Fellow

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
Wolfson College

Emeritus Reader in Electronic Materials
OCAMAC Senior Fellow

Studies of semiconductor materials and devices. Group III-V's, Si and SiGe. Ingots, single and multiple layers, superlattices, quantum wells and dots,. Single crystals, polycrystalline and amorphous layer. Composition, geometry, interfaces, defects, phase separation, atomic ordering. Relationship between growth method, processing conditions, structures, optical and electrical properties. Lasers, detectors, MOSFETS, bipolar transistors.



Professor Andrew Briggs
Wolfson College

Professor of Materials

Nanostructures and surfaces. Design and characterisation of nanocomposites for packaging. Semiconductor nanomaterials for electronics and quantum computation.

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



Professor Richard Brook OBE FREng
St Cross College

Professor of Materials

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.



Professor Brian Cantor FEng
St Catherine's College

Cookson Professor of Materials
Head of Division of
Mathematical and Physical Sciences

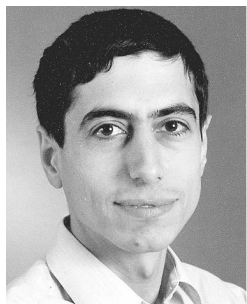
Relationship between manufacture, microstructure and properties of engineering materials, in particular metallurgical alloys, metal matrix composites, wear and corrosion resistant coatings and thin film functional metals, ceramics and composites, particularly associated with the aerospace, automotive and packaging industries.

- Rosenhain Medal and Prize, Institute of Materials, 1993

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.



Dr. Alfred Cerezo
Wolfson College

Reader in Materials

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**
Linacre College **Physical Examination of Materials**

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.



Dr. John Coyle FRSC
Linacre College

OCAMAC Senior Fellow
Linacre College Industrial Fellow

Role of technology and innovation in small and medium-sized enterprises, and the processes of forming beneficial links between such companies and the 'knowledge base' including university departments and other research laboratories.



Dr. Jan Czernuszka
Trinity College

Lecturer in Materials

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

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



Professor Brian Eyre CBE FEng. FRS
Wolfson College

Visiting Professor
Wolfson College Industrial Fellow

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

[Retired as Chairman of CLRC, running the Daresbury and Rutherford Appleton Laboratories on 30 September 2001]



Dr. Patrick Grant
Linacre College

Reader in Materials
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. Geoff Grime

University Research Lecturer

Development of techniques for materials characterisation using focused MeV ion beams, in particular the design of high resolution focusing systems for high energy ions and data acquisition and processing systems. Application of these techniques to a wide range of scientific disciplines.



Dr. Chris Grovenor
St Anne's College

Reader in Materials
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
St Edmund Hall

Emeritus Professor

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
St Edmund Hall

Professor of Physical Metallurgy

Modelling and understanding fundamental solidification processes. This has included 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.
- The C.H. Mathewson Gold Medal. TMS AIME. 1967

Dr. John Hutchison
Wolfson College

Reader in Materials

Development of high resolution electron microscopy for structural characterisation of new materials including : CVD diamond films, quantum dots, inorganic fullerenes and complex oxides. Development of controlled environment electron microscopy for in-situ study of catalysts and of gas-solid reactions. Other interests include novel forms of carbon e.g. nanotubes.

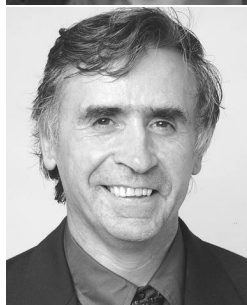
- Glauert Medal, Royal Microscopical Society, 1975
- Vice President of the Royal Microscopical Society, 2000



Dr. Beverley Inkson
St Edmund Hall

Royal Society University Research Fellow

Mechanical properties and wear of nanostructured materials. Nanotribology. Mechanisms of deformation and failure in 'spatially confined' nanostructured systems including nanocomposites, multilayered devices and thin film coatings. Techniques used include nanoindentation, in-situ mechanical testing in electron microscopes, and 3D microstructural analysis by FIB.



Dr. Mike Jenkins
Jesus College

Reader in Materials

Director of Electron Microscope Facilities

Radiation damage, transmission electron microscopy, phase stability under irradiation. 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. Oleg Kolosov
Wolfson College

EPSRC Advanced Fellow

Elastic and visco-elastic microstructure of materials, particularly ceramics, glasses, semiconductor quantum structures, polymer nanocomposites. Development of ultrasonic and scanned probe microscopy techniques for imaging and characterisation of surface and subsurface elastic and non-mechanical properties of materials on the micro and nanoscale. Nanoscale dynamics of ferroelectric domains.

- Metrology award for World Class Manufacturing, 1999



Dr. John Martin
St Catherine's College

**Emeritus Reader
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. Günter Möbus

EPSRC Advanced Fellow

Characterisation of materials on the atomic and nano-scale. Development of tomography techniques for 3D composition mapping and solving of crystal defect structures by high-resolution electron microscopy in combination with analytical TEM. Advanced studies on statistical image processing and dynamical simulations of electron diffraction.



Dr. Christiane Nörenberg
Wolfson College

Royal Society Dorothy Hodgkin Fellow

Growth of quantum nitride nanostructures (InGaN, AlGaIn) by molecular beam epitaxy (MBE) and in-situ surface characterisation 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 composition and growth parameters.



Dr. Peter Northover
St Catherine's College

Lecturer in Materials

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
The Queen's College

Lecturer in Materials

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 Chris Peel

Visiting Professor

Director of Technology for Future Systems technologies QinetiQ looking after all aspects of future technology for platforms, systems appropriate and their supporting technologies such as materials and structures. Specific expertise in aerospace structural materials.



Dr. Amanda Petford-Long C.Phys, M.Inst.P.
Corpus Christi College

Reader in Materials

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.

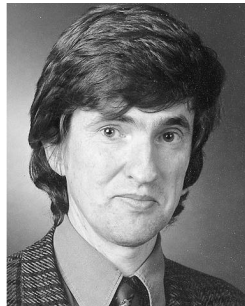


Professor John Pethica FRS
St Cross College

Visiting Professor

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.

- Hughes Medal, The Royal Society, 2001.
- Rosenhain Medal and Prize, 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

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

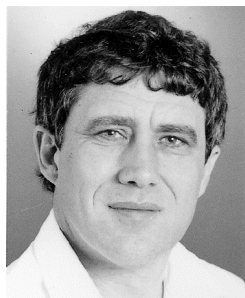
- Royal Society Armourers and Brasiers' Medal 1999
- William Hume-Rothery Award, TMS 1995.
- Hume Rothery Prize, Institute of Materials, 1990.



Dr. Rosetta Plummer
St Edmund Hall

Department Administrator

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
St Cross College

Reader in Materials

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. Oleg Salata

OCAMAC Senior Research Fellow

Organic Electroluminescence: novel emissive and charge transporting materials, their characterisation and optimisation. Design and fabrication of organic light emitting devices(OLEDs), modelling of device characteristics. Effects of material properties, chemical structure and thin film morphology on device performance and stability. Advanced fabrication techniques for OLEDs and OLED based displays. Engineering of organo-inorganic interfaces for improved OLED performance.



Dr. Peter Schumacher

EPSRC Advanced Fellow

Mechanisms and kinetics of heterogeneous nucleation in metallic alloys and the mechanisms by which grain refiner additions operate, including direct transmission electron microscope observation of the devitrification of metallic glasses to observe discrete nucleation events.

- Cook Ablet Award, Institute of Materials, 2000



Dr. Jeremy Sloan
Wolfson College

Royal Society University Research Fellow
(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
Trinity College

Professor of Materials
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 FInstP, FIM **Professor of Materials Science**
Linacre College **Director of the Materials Modelling Laboratory**

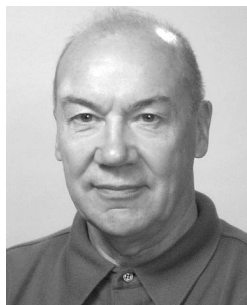
Modelling of materials at the atomic and microstructural levels. Adhesion of polymers to inorganic substrates. Mechanical, thermal and electrical properties of metallic nanocontacts. Electromigration. Long-range elastic interactions and microstructural evolution due to diffusional phase transformations. Microstructural damage and evolution in fusion reactor materials. Long-standing interest in interfaces.



Dr. John Sykes
Mansfield College

Reader in Materials

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



Dr. Glyn Taylor
Linacre College

Senior Research Fellow

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
St Anne's College

**RAE Research Professorship in
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
St Catherine's College

Lecturer in Materials

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.



Dr. Drahosh Vesely
Wolfson College

OCAMAC Senior Fellow

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



Dr. Tiffany Walsh
Linacre College

Glasstone Research Fellow

Modelling interfaces between hard and soft matter at atomic and mesoscopic levels. Efficient implementation of perturbation theory in periodic systems. Development of techniques to accurately calculate weak interactions between molecules and metal surfaces. Modelling adhesion of polymers to inorganic substrates. Modelling of self-assembled monolayers on inorganic surfaces.



Professor Mike Whelan
Linacre College

Emeritus Professor

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
Corpus Christi College

**Royal Society University Research Fellow
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
St Anne's College

Lecturer in Materials

Characterisation of the electrical and mechanical properties of defects in semiconductors. High resolution 2D mapping of dopant distributions in semiconductors. Development of novel structures and materials for field emitters to be used in field emitter displays. Improved biomaterials for prostheses.



Professor John Wood

**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 - INTERMETALLICS

Mechanical Properties of γ -TiAl

N. Bird, Dr. S. Jiao*, Professor Sir Peter Hirsch, Dr. G. Taylor

Single crystals of γ -Ti 54.5% Al with various orientations have been deformed over a range of temperatures, and the dislocation structures analysed by TEM. Mechanisms are being developed to explore the yield stress anomalies observed for slip on $1/2\langle 110 \rangle\{111\}$, $1/2\langle 112 \rangle\{111\}$ and $\langle 011 \rangle\{111\}$ systems, and why the yield stress for $\langle 011 \rangle\{111\}$ slip is reversible with temperature, but that for $1/2\langle 110 \rangle\{111\}$ slip is not. (*Argonne National Laboratory, Argonne IL, USA) (Funded by EPSRC and QinetiQ Pyestock)

3D microstructural characterisation of intermetallics

Dr. B.J. Inkson, Dr. M. Bobji, Dr. P. Threadgill*, Professor H. Clemens**

The 3D microstructures of TiAl and FeAl intermetallics, processed by rolling and friction welding, are being determined by a new technique of 3D FIB analysis, combined with TEM and EBSD. This enables the grain shapes and orientations in 3D to be directly correlated with local mechanical properties across non-uniform microstructural features. (*The Welding Institute, Cambridge; **GKSS Germany)

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. The mechanical properties of the ternary alloys will be measured and the associated dislocation structures characterised by electron microscopy.

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)

Transition metals in TiAl

Dr. K. Xia*, Dr. B. Inkson, Professor B. Cantor

Microstructures of $\gamma + \beta + B2$ Ti - Al alloys are being examined as a function of processing conditions and ternary alloying additions at the atomic scale using high resolution chemical and structural electron microscopy analysis techniques. (*University of Melbourne, Australia)

Growth of single crystals and deformation characteristics of binary RuAl and other B2 alloys

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

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 is being constructed for operation at above ambient pressure in an attempt to grow good quality crystals of RuAl and other B2 intermetallic compounds. The mechanical properties of the crystals will then be studied by a variety of methods and dislocation structures characterised by transmission electron microscopy.

Dislocation dipoles in γ -TiAl

Professor Sir Peter Hirsch

Faulted dislocation dipoles are a common feature of the deformation of γ -TiAl at low temperatures. A new model is being developed to explain the formation of these defects.

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

Dr. A.L.R. Sabariz, 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.

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 $1/2[112]$ dislocations in γ -TiAl are being simulated using the CUFOUR programme with a view to distinguishing between possible alternative structures of these defects.

II - NANOCRYSTALLINE MATERIALS

Metallic nanocrystalline materials

M. Abraham, Dr. A. Cerezo, Professor G.D.W. Smith

Electrodeposition is being investigated as a possible method for the production of single phase, multiphase and alloy nanocrystalline materials. Apart from its simplicity, this method has the advantage that it can produce large quantities of material without the need for subsequent consolidation. However, the alloy compositions need to be chosen to produce a microstructure which resists rapid grain growth during service. Nickel- and iron-based alloys produced by electrodeposition are being characterised by X-ray diffraction, TEM and field-ion microscopy/atom probe techniques. (Funded by EPSRC in collaboration with Carpenter Technology)

Microstructure and mechanical properties of thin films and nanowires

Dr. B.J. Inkson, Dr. M.S. Bobji, Professor E. Arzt, Dr. G. Dehm*, Dr. Th. Wagner*, Dr. O. Kraft**

High strength multilayered thin-films, grown on ceramic substrates by molecular beam epitaxy (MBE), are subjected to controlled static (indentation) and cyclic (thermal and stress) mechanical deformation. The resulting evolution of the thin film microstructures are quantified by 3D FIB and electron microscopy down to the atomic level. (*Max-Planck-Institut für Metallforschung, Stuttgart, Germany) (Funded by The British Council, DAAD and The Royal Society)

FIB characterisation of surface damage generated by nanoindentation, scratch testing and abrasion

T. Steer, Dr. H. Wu, P. Boon, Dr. M.S. Bobji, Dr. B.J. Inkson

Surface plastic deformation in multilayers and nanocomposites, generated by nanoindentation, scratch tests and abrasion, are being systematically characterised by high resolution electron microscopy and 3D FIB. (Funded by EPSRC and The Royal Society)

Nanoscale deformation of materials quantified by TEM nanoindentation

Dr. M.S. Bobji, Dr. B.J. Inkson, Professor J.B. Pethica, R.C. Doole*

A novel nanoindenter is being built to enable the impact and deformation of nanostructured materials to be observed in real time inside a TEM down to the atomic level. Mechanisms of deformation will be correlated to the applied load, indenter morphology, substrate microstructure and chemistry. (*Trinity College, Dublin) (Funded by EPSRC and The Royal Society)

Microstructure-strength relationship of novel metallic nanocomposites studied by 3D analytical TEM

S.H. Kim, G. Möbus, B.J. Inkson

We use electron spectroscopic tomography techniques to study the microstructure and elemental distribution of nanocomposite alloys on a nm-scale. Materials comprise quasicrystalline particle reinforced Mg-base alloys and metallic glass/precipitate composites. (Funded by KOSEF and in collaboration with Yonsei University, Korea)

III - MECHANICAL PROPERTIES OF STRONG SOLIDS, METALS AND ALLOYS

Microstructure and mechanical properties of 7xxx and 8xxx alloys

Dr. I.G. Palmer, Professor B. Cantor

Electron microscopy, heat treatment and mechanical testing methods are being used to investigate the microstructure and static and cyclic mechanical properties of 7xxx and 8xxx alloys. The results are being used to optimise the materials for applications in airframe and other components. (Funded by QinetiQ)

Short Fatigue Crack Growth in Al-Li alloys

C. Gourlay, Dr. J.W. Martin, Dr. A.J. Wilkinson, Dr. G.R. Davis, Professor J.C. Elliott**

The effects of local grain size and orientation on the growth rate of short fatigue cracks in Al-Li alloys is being examined. Electron back scatter diffraction allows grain orientations along the crack path to be determined. We will also explore the use of X-ray micro-tomography in studying the changes in the three dimensional geometry of fatigue cracks as a function of number of applied load cycles. (*Biophysics in Relation to Dentistry, Queen Mary and Westfield College, London)(Funded by EPSRC through JREI scheme)

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)

Growth of short fatigue cracks in nickel based superalloys

*Dr. A.J. Wilkinson, Dr. J.W. Martin, Dr. P.A.S. Reed**

The growth of short fatigue cracks in polycrystalline nickel based superalloy turbine disc material is to be studied. Experiments will correlate measured local fluctuations in growth rates with the path taken by short fatigue cracks through the microstructure. Physically based models of multiply deflected cracks will be developed and used to simulate the effects of grain size and orientation distributions on the statistics of the early stages of crack growth. (*Materials Research Group, University of Southampton). (In collaboration with Alstom and QinetiQ)

Characterisation of cold worked microstructures in aluminium alloys

*N.J. Akram, Dr. R.I. Todd, Professor F.J. Humphreys**

The main aim of the project is to use X-ray diffraction peak broadening to characterise cold worked microstructures which are too dense and complex to be resolved in the TEM. Previously developed analysis methods will be adapted and tested using simple alloys with microstructures which can be characterised by alternative methods. Complementary techniques such as measurement of the thermoelectric effect will also be included in the investigation. (*UMIST) (Funded by EPSRC and Alcan International Ltd.)

Microstructure-property relationships in commercial superplastic 7475-aluminium alloys

*Dr. D. Whittle, Dr. R.I. Todd, Dr. N. Ridley**

The microstructural features controlling flow stress and cavity nucleation during superplastic forming of commercial 7475-Al alloys are being investigated. The microstructures of material deformed using both conventional uniaxial deformation and sheet forming of cones are being examined using FEG-SEM and EBSD. The influence of back pressure on cavitation is also being revisited. (*University of Manchester) (Funded by British Aerospace Military Aircraft & Aerostructures)

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 70 at% 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. J.W. Martin

Single crystal specimens are being tested in fatigue under constant plastic strain amplitude conditions. The dislocation microstructures produced are being examined using electron channelling contrast imaging, a novel SEM technique, and their evolution is being modelled by computer simulation. The objective is an understanding of dislocation patterning and subsequent initiation and early growth of fatigue cracks.

Carbide cracking and the brittle-ductile transition in ferritic steels

M. Coates, Dr. A. J. Wilkinson, Dr. S.G. Roberts

The effect of brittle carbides on the fracture behaviour and brittle-ductile transition in ferrite is being studied experimentally, and the evolution of dislocation arrays around crack tips and these particles is being modelled. The objectives are to understand the basic processes leading to cleavage fracture in steels, and hence to underpin the FEM-based models used in safety codes (Funded by EPSRC in collaboration with AEA Technology, HSE and NII)

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 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.

Fundamentals of Fatigue Crack Initiation in Nickel based Superalloy

J. Buckley, Dr. J.W. Martin, Dr. A.J. Wilkinson

Single crystals of SRR99 of differing orientation will be tested under fatigue loading. The evolution of 'damage' in the crystal will be monitored through SEM observation using electron channelling contrast imaging. The localisation of surface roughening into intrusions, extrusions and the subsequent formation and growth of cracks will be studied. We aim to explore the effects of mode mixity (modes I and II) and compare single and multiple slip configurations.

Cooperative Nucleation of Shear Dislocation Loops

Professor Sir Peter Hirsch, Dr. Y.Q. Sun*, Dr. P.M. Hazzledine**

The mean elastic interaction between subcritical shear loops is the "image stress", which leads to the cooperative nucleation of such loops, resulting in a transition temperature, above which stable expanding loops are generated. The magnitude of this effect is being assessed. (*Department of Materials Science and Engineering, University of Illinois; **Air Force Research Laboratory, Wright-Patterson AFB, Dayton, Ohio)

Mechanical properties and microstructural evolution of semi-solid slurries

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 the Al alloy automotive components.

Development of corrosion resistant high strength ferritic steels

Professor J.M. Titchmarsh, Dr. P. Schumacher, 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)

B. Non-Metallic Materials

I - CERAMICS AND COMPOSITES

Nanocomposite ceramics for technical applications

P. Boon, Dr. A.M. Cock, Dr. S.G. Roberts, Dr. R.I. Todd, Dr. B.J. Inkson, 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.

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 SiO₂ 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)

Ultrahard multilayered ceramic coatings

*T. Steer, Dr. B.J. Inkson, Dr. K. Cooke**

Mechanisms of improvements in mechanical strength achieved by grain size reductions and lamellar spacing of nitride and boride ceramic multilayers are being quantified using indentation, cross-sectional TEM studies and HREM. (*Teer Coatings Ltd.) (Funded by EPSRC)

Abrasion mechanisms of alumina

Dr. B.J. Inkson, Dr. G. Möbus

The abrasion mechanisms of alumina are being studied at the atomic scale. High resolution cross-sectional electron microscopy studies of abraded surfaces are being carried out to resolve the structure of deformation twins and dislocation core structures.

Surface mechanical properties of alumina/SiC nanocomposites

J.L. Ortiz Merino, Dr. R.I. Todd

Previous work has shown that the addition of a small volume fraction of nanoscale SiC particles to a conventional alumina matrix can significantly strengthen the alumina grain boundaries. One manifestation of this effect is a dramatic reduction of the surface grain pullout during surface abrasion which is prevalent in unreinforced alumina. This leads to improved surface finish and wear resistance. The reason for the grain boundary strengthening is being investigated by studying the response of alumina matrix nanocomposite surfaces to abrasion as key microstructural features (grain size, particle size, particle location, particle properties) are varied systematically. (Funded by the Mexican Government)

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)

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. (In collaboration with Hardide Ltd.)

High temperature strengthening of zirconia ceramics

R. Kathuria, 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 high strength at high temperature.

GAP - A Ceramic Extraordinaire?

I. Shapiro, Dr. R.I. Todd

Recently published results have suggested that gadolinium aluminium perovskite (GAP) has remarkably good mechanical properties (e.g. $K_{Ic}=10\text{MPam}^{0.5}$). The details are sketchy, and the toughening mechanism unknown. The aim is to make some GAP and study its properties in detail.

II - BIOMEDICAL MATERIALS

Crystallographic texture determination of calcium phosphates

Dr. P. Fewster*, Dr. P. Kidd*, 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)

Bone biomaterials bonding

Dr. J.T. Czernuszka, Professor J.J. O'Connor*

The micromechanical properties of the biomaterial/long bone interface are being measured. This allows us to measure externally the incorporation rates of the biomaterial. (*Oxford Orthopaedic Engineering Unit)

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)

Mechanical properties of biocomposites

D. Gatora, Dr. D. Vesely, 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.

Macro-assembled spheres of apatite

O. King, T. Pongsaanutin, 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. (Funded by Wellcome Trust, Thai Government, EPSRC, AEA Technology)

In vitro approaches to bone formation

Dr. J.T. Triffitt*, Dr. J.T. Czernuszka, S. Wilkinson

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.)

Nanolaminated composites

Dr. J.T. Czernuszka

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

Modelling phospholipid monolayers at the alveolar interface

Dr. I. Gentle, K. Gunton*, 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)

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, M. Karlsson, Dr. E. Palsgard*, Dr. L. di Silvio**, 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. (*Centre for surface biotechnology, Uppsala University, Sweden; **UCL, UK)

Structure and properties of silk

*J. Trancik, 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) (Funded by The Rhodes Trust)

Characterisation of spider silk and spin glands

Dr. F. Vollrath, Dr. D. Knight, Dr. G.W. Grime*

Spider silk and spin glands are being characterised using micro-PIXE imaging to investigate the role of trace elements such as Ca and Zn in the production of these materials.

3D Microstructure of Bio-Nanomaterials

Dr. P. Vukusic, Dr. G. Möbus*

We are developing electron tomography techniques to characterize in 3D the structural units, periodic lattice, and defects of naturally grown nanostructured materials. (*University of Exeter)

Three Dimensional Scaffolds for Tissue Engineering

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

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

III - POLYMERS

Coated Steel

Dr. K. Porfyraakis, Dr. H.E. Assender

Investigation of surface morphology of polymer coatings on steel by ATR-FTIR scanning probe microscopy. (In collaboration with Corus with funding from Corus).

Fabrication of micro-optical components using MeV ion beam lithography

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

Direct write ion beam lithography is being investigated as a method of fabricating micro-optical components (gratings, waveguides, etc.) for use in optical communications devices.

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)

Development of ion-permeable membranes

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

Various chemical and physical treatments may be applied to ion-permeable membranes to modify their performance. Such developments are attempted and characterised in terms of the extent and nature of the modification. (Funded by EPSRC and Regenesys)

Creep, fatigue and environmental stress cracking of polymers

Dr. R. Matthews, Dr. D. Vesely

Crack propagation under different types of loading of polyethylene samples in an oxidative environment is investigated. The response of the polymer to stress concentration is critically dependent on the physical and chemical state of the microstructure. The conditions for acceleration or deceleration of the crack propagation are being established. (Funded by National Power)

Diffusion and solubility in polymers

L. Castro Diaz, G. Bernardo, Dr. D. Vesely,

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

Diffusion in composite materials

M. Zhu, Dr. H.E. Assender, Dr. D. Vesely

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.

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 charged 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)

Oxidative degradation of polymers

T. Burman, Dr. H.E. Assender, Dr. D. Vesely

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 EPSRC and Regenesys)

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.

Mechanical properties of polymer interfaces

Dr. R. Matthews, Dr. D. Vesely

Molecular interactions and entanglement at interfaces of homo-polymers and polymer blends are investigated and correlated with interfacial fracture. Stress distribution at interfaces with different microstructure are studied by finite element analysis with the aim to establish the conditions for the formation of microcracks. The results are applied to the mechanical behaviour of polymer welds, polymer blends and composites. (Funded by National Power)

Gloss of polymers

Dr. K. Porfyrikis, 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.

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)

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

M. Moniruzzaman, 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, T_g , 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 microstructure on the mechanical properties of polymer systems and composites.

Molecular Structure of Nanotubes Derived from Polyrotaxanes

Dr. D.G. Bucknall, M. Waring

Using a combination of techniques we are studying the structure of nanotubes derived from polyrotaxane molecules. These tubes have tube dimensions which are dependent not only on the macrocycle used to thread the polymer to form the polyrotaxane, but also on the molecular weight of the initial polymer. We will use a number of techniques to study these molecules including, small angle neutron scattering, STM and high resolution electron microscopy.

Interfacial Failure Mechanism in Polymer-Ceramic-Metal Composites

*Dr. D.G. Bucknall, T. Bromwich, Dr. P. Short**

Power line surge arresters are made from ceramic and metal sandwiches wrapped in polymer for strength and environmental protection. During testing samples can fail by the polymer coating unwrapping. This project is undertaking a detailed study of polymer-non-polymer interfaces under extreme conditions as may be experienced under extremely high temperatures and fields for short periods of time. (*Bowthorpe EMP)

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.

Investigation of rapid radiation induced decomposition of PTFE for micromachining applications

Dr. G.W. Grime, Dr. C.J. Sofield

Polymers such as PTFE have been observed to decompose rapidly to gaseous products under bombardment with MeV heavy ions (e.g. 2MeV Ar). This process is being investigated theoretically and experimentally as a unique method of fabricating very high aspect ratio microstructures in PTFE either by direct writing with a focused beam or by masking in a broad beam.

IV - PACKAGING MATERIALS

Characterisation of glassy barrier films on PET substrates

Dr. B.M. Henry, G. Erlat, Dr. C.R.M. Grovenor, Dr. G.W. Grime

The microstructure of PET/glass films is being studied in order to correlate the gas transmission properties with structures intrinsic to the glassy layer and defects produced during fabrication and handling. High resolution TEM and SEM, Atomic Force Microscopy and microanalysis techniques such as SIMS and the Scanning Proton Microprobe are being used to study the structure and composition of the glass layer. Observations of defects such as local cracking, porosity and the analysis of chemical reactions with water are proving valuable in explaining the barrier layer properties of these composite packaging materials. (Funded by and in collaboration with The Toppan Printing Company)

Prediction and measurement of crystallinity at a polymer surface

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

An algorithm has been developed for the quantitative comparison of ATR-FTIR data with transmission FTIR data, to enable the quantitative measurement of the surface properties of polymers. The crystallinity and molecular orientation towards the surface of a polymer is measured after a range of thermal treatments and mechanical deformation of the material. (Funded by The Toppan Printing Company)

Deposition of novel glassy barrier layers for packaging applications

G. Erlat, Dr. C.R.M. Grovenor, Professor R. Howson and Dr. B.M. Henry

Reactive, dual target sputtering is being used to deposit Al(X) oxynitride films of carefully controlled composition in order to investigate the feasibility of improving barrier layer properties by the formation of highly dense oxide films. The permeation of water vapour and oxygen through these barrier films is being measured and correlated with microstructural observations. Of particular interest is to develop an understanding of the permeation mechanism of water vapour through these composite samples. (Funded by and in collaboration with The Toppan Printing Company)

Design and characterization of layered nanocomposite materials

*Professor G.A.D. Briggs, Professor G.D.W. Smith, Professor A.P. Sutton, Dr. C.R.M. Grovenor, Dr. O.V. Kolosov, Dr. H.E. Assender, Dr. Y. Tsukahara**

Layered nanocomposite materials are used to provide enhanced gas barrier properties for food packaging and other applications. We study the structure of such materials and the mechanisms of gas permeation, with a view to understanding their properties and designing materials with enhanced performance. Individual projects include characterization by electron microscopy and secondary ion mass spectroscopy, imaging and measuring nanoscale mechanical properties and local gas transmission, polymer surfaces and interlayers, and theoretical modelling of oxide film formation. (*Toppan Printing Company Ltd) (Funded by The Toppan Printing Company)

Development of a prototype gas transmission microscope

Dr. H. Norenberg, Professor G.D.W. Smith, Professor G.A.D. Briggs

A gas transmission microscope is being developed to study gas permeation through thin barrier films with high spatial resolution (at the micron level). This instrument will be used to correlate the microstructure of the barrier layers directly with the local transmissivity. (Funded by and in collaboration with The Toppan Printing Company)

Deposition and characterisation of nanoporous conducting oxide films

Dr. B.M. Henry, G. Erlat, A.O. Cornick, M.F.D. Winch, 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 is using sputtering, sol-gel and electrophoretic deposition to fabricate TiO_x thin films with controlled porosity. 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 and AFM. (Funded by and in collaboration with The Toppan Printing Company)

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.

Fabrication of thin films of superconducting ceramics

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

Sputtering and post annealing processes are being used to deposit thin films up to 3" 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 Cambridge, Department of Physics, Imperial College.)

Microwave device fabrication from superconducting thin films

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

Prototype passive microwave components (filters, resonators, mixers and correlators) are being fabricated in 2 inch diameter TlBaCaCuO thin films on LaAlO₃ substrates, and their performance compared with superconducting properties to optimise preparation processes. World class surface resistance values are routinely achieved, and a range of novel device types are being studied particularly for applications in digital TV systems. More fundamental properties of thin films containing an array of defects are also being investigated. (Funded by EPSRC and in collaboration with WSIL Ltd, BBC, Hymatic Ltd., University College London and Department of Engineering Science*)

Development of novel metallic substrates for superconducting tapes

R.M. Whiteley, Dr. J. Moore (now in Univ. Munich), Dr. C.R.M. Grovenor, Dr. J.M. Sykes

The thermal/mechanical properties of silver and silver alloy substrates have been 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 YBaCuO superconductor layers by a wide range of techniques. In Oxford, the crystallographic relationship between the metal substrate and the superconducting phase is a central aspect of our work, and is analysed by texture X-ray diffractometry and EBSD. (Funded by EPSRC and in collaboration with Advent Research Materials Ltd., Department of Metallurgy, University of Cambridge and NREL, USA)

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

R.M. Whiteley, Dr. J. Moore (now in Univ. Munich), 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, Ag/Rh/Ni buffer layer combinations in order to demonstrate the compatibility of these structures with in-situ deposited superconducting layers. At the same time, the fundamental processes that operate in the phenomenon of electroepitaxy are being investigated.

Development of practical conductors and devices from high temperature superconducting ceramics

Dr. J.C. Moore(now in Univ. Munich), Dr. C.R.M. Grovenor, Dr. M. McCulloch*, Professor D. Dew-Hughes*

Several fabrication routes are being used to produce from superconducting ceramic materials prototype conductors capable of carrying significant currents at liquid nitrogen temperatures and much larger currents at lower temperatures. Current work is concentrating on the development of dip coating deposition techniques. 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 properties. The ways in which these conductors may be fabricated into useful devices, such as magnets motors and fault current limiters, are being investigated and demonstrator devices produced and tested. Superconductor systems based on Bi, Tl and Hg are all under investigation. (*Department of Engineering Science) (Funded by EPSRC)

Microstructural characterisation of superconducting materials

Dr. H. Wu, S. Speller, C.J. Dark, C.J. Salter, Dr. G. Grime, Dr. C.R.M. Grovenor

Superconducting ceramic samples fabricated in bulk and thin film 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, electron microprobe proton microprobe and orientation imaging microscopy techniques are being used to study the key microstructural features. (Funded by EPSRC and in collaboration with Oxford Instruments, University College London, Cambridge University and Imperial College, London.)

II - SEMICONDUCTOR MATERIALS

Polysilicon emitter bipolar transistors

Dr. C.D. Marsh, Dr. G.R. Booker, Dr. C.R.M. Grovenor, Dr. G. Nash*, Dr. J.F.W. Schiz*, Professor P. Ashburn*, Dr. P. Osborne**, Professor D.J. Roulston***

Polysilicon layers are deposited on silicon wafers, implanted with arsenic and annealed. The effects of incorporated fluorine on interfacial oxide break-up and polysilicon layer regrowth are determined using TEM, SIMS and electrical measurements. Application to high performance polysilicon emitter bipolar transistors. (*Electronics Department, Southampton University; **Zarlink Inc., Swindon; ***Electrical Engineering Department, Waterloo University, Canada)

Dopant profiling in silicon by chemical etching, TEM and AFM

K.D. Yoo, Dr. C.D. Marsh, Dr. G.R. Booker, Dr. C.R.M. Grovenor

One dimension and two dimension dopant profiles are being determined in implanted and annealed bulk silicon wafers and MOS transistors by using selective chemical etching in combination with AFM and TEM techniques. The method is being developed for application to shallow p-n junction devices.

Investigation of strain distributions in semiconductors

Dr. A.J. Wilkinson

A techniques 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. (Funded by The Royal Society)

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.

Physical embodiment of qubits

M.R. Austwick, Professor G.A.D. Briggs

We shall investigate the physics of candidate systems for embodying qubits in a solid state quantum logic gate.

Impurities and dislocations in Si wafers

Dr. S. Senkader, A. Giannattasio, 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 350-700°C 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)

Quantum dots

S. Booth, 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.

Quantum wires and dots

Dr. J.L. Hutchison, S. Gledhill, N. Allsop, Professor P.J. Dobson, R.N. Taylor, Dr. O.V. Salata, 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. (*Department of Engineering Science; **Nanox Ltd.)

Improved Si substrates for microwave applications

Dr. K. Mallik, Dr. S. Senkader, Dr. R. Falster, Dr. P.R. Wilshaw*

This project is to investigate materials issues that affect the speed of integrated circuits processed on silicon or silicon based structures and to develop strategies for producing improved materials. Novel methods are being investigated and microwave test structures will be fabricated. (*MEMC, Italy) (Funded by MEMC)

Room temperature light emission from 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)

Nanoelectronics at the Quantum Edge

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

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. (*Department of Physics; **Microelectronics Research Centre, Department of Physics, Cambridge University; ***Hitachi Cambridge Laboratory, Hitachi Europe Ltd.) (Funded by Foresight LINK Project, DTi and Hitachi Europe Ltd)

III - MAGNETIC MATERIALS

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

Dr. A.K. Petford-Long, Dr. Y. Wang, Dr. H. Laidler, Professor K. O'Grady**

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. (*Univ. of York) (Funded by EPSRC and Seagate Technology)

Studies of patterned magnetic thin films

Dr. R. Langford, N.W. Owen, Dr. 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. Their 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)

Spin-tunnel junctions based on magnetic layered films

Dr. A.K. Petford-Long, Dr. D. Ozkaya, Dr. B. Warot, 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 via a collaboration with the Univ. of Cambridge and Univ. of Plymouth)

Effect of pinning layer material in spin-valve materials

A.R. de Morais, Dr. A.K. Petford-Long, Dr. A. Cerezo

The effect of different pinning layer materials on the magnetic and transport properties of NiFe-based spin-valve structures is being studied. The films are being grown by sputter-deposition and electron microscopy techniques are being used to assess their properties. (In collaboration with Nordiko Ltd.)

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

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

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)

Composite magnetic nanoparticle systems

A. Eggeman, Dr. A.K. Petford-Long, Professor P.J. Dobson

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

IV - DISPLAY MATERIALS

Non-lithographic definition of sub-micron field emitter structures

Dr. J. Kang, A. Weardon, Professor V. Baranauskas, Dr. P.R. Wilshaw

At present most triode type vacuum microelectronic devices are fabricated using sub-micron resolution lithography. Such processing is costly and difficult to achieve over the large areas required for field emitter displays. This project involves the use of specially fabricated materials which contain sub-micron features suitable for field emission without the need for lithographic processing. (Funded by EPSRC)

Dendrimers as multifunctional materials for OLEDs

Dr. H. Mustafa, Dr. P. Burn**, Dr. I.D.W. Samuel***, Dr. O.V. Salata*

Dendrimers or starburst molecules have been applied recently to both light emitting and charge transporting layers in OLEDs. It is possible to design dendrimeric molecules that can direct both charge and energy to the light-emitting moiety. If this light-emitting moiety is a lanthanide ion then a pure emission is expected. The objective of this project is to find out the “design rules” of the efficient electroluminescent molecules possessing bipolar transport abilities. We are trying to establish relations between molecular structure and behaviour of dendrimers in electroluminescent devices. (*Opsys Limited; **DPL, Department of Chemistry; ***Department of Physics, St Andrews University) (Funded by Opsys Ltd.)

Development of electroluminescent display based on phosphorescent materials

D. Mathieson, Dr. V. Christou, Dr. O.V. Salata*

Phosphorescent molecules are promising electroluminescent materials that can be used in flat panel displays. Their fundamental advantages such as utilisation of the triplet excitations in light generation make these materials favourite candidates for the future displays. Advanced light-emitting and charge-transporting materials are under constant development at ICL, University of Oxford. Organic light-emitting devices based on those novel materials are optimised for the highest possible performance. (*ICL, Department of Chemistry) (Funded by Opsys Ltd.)

Material issues in degradation of OLEDs

Dr. V. Christou, Dr. O.V. Salata*

Although reports on the long operational lifetime of the OLEDs are not uncommon, most of them are referred to the TPD/Alq₃ based devices. It is expected that organolanthanide based devices should possess an improved stability. However, no experimental information is yet available to support this claim. The objective of this project is to establish the influence of environmental factors like oxygen and moisture as well as charge transport and heat dissipation on the degradation of organolanthanide based OLEDs. Established molecular structure-stability dependencies will allow us to design more robust molecules. (*ICL, Department of Chemistry)(Funded by Opsys Ltd.)

Carbon nanotube field emission displays

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

Field emitting structures based on carbon nanotubes embedded in an alumina matrix are being investigated. These show potential for large area display devices with a gate structure simply integrated into the cathode emitting region. (Funded by EPSRC)

OLED interface engineering using ultra-thin inorganic layers

Dr. Z. Liu, Dr. O.V. Salata

Typical OLED device contains a number of interfaces both organic-organic and organic inorganic. These interfaces quite often control the charge balance and hence device efficiency. Various deposition techniques of ultra-thin inorganic layers are used to create tunnelling layers located at different interfaces. Morphology of the resulting layers is studied using AFM and related methods and is linked both to the deposition conditions and device performance. (Funded by Opsys Ltd.)

Studies of field emitter/phosphor interactions for display applications

Dr. M. Ushirozawa, Dr. A. Cerezo, Professor P.J. Dobson, Professor G.D.W. Smith*

Field emission microscopy and atom probe microanalysis techniques are being combined to study the degradation mechanisms in field emitter displays. (*NHK, Japan) (In collaboration with NHK, Japan and Nanox Ltd., Oxford)

D. Processing

Freeform fabrication of ceramics and metals using ink-jet printing

N. Reis, K. Seerden, Dr. P.S. Grant, Dr. B. Derby*, Dr. J. Evans***

It is possible to construct rapid prototypes of complex engineering structures slice by slice using 3-dimensional printing technology. We are developing ceramic suspensions in low melting point waxes for drop-on-demand ink-jet printing of 3D shapes. (*University of Manchester; **Queen Mary and Westfield College) (Funded by EPSRC)

The downstream processing of twin roll cast aluminium alloys

*Dr. M. Yun, Dr. C. Gras, Professor J.D. Hunt, Dr. K.M. Gatenby**

The solidification conditions experienced during twin roll casting result are very different from those in conventional direct chill (D.C.) cast ingots. This project is concerned with how these differences affect the final properties of twin roll cast aluminium sheet after downstream processing. (*Alcan International) (Funded by EPSRC and Alcan International)

Twin roll casting of stainless steel and other ferrous alloys

Dr. M. Yun, Professor J.D. Hunt

The twin roll casting of ferrous alloys is of great commercial interest, to date the majority of research has concentrated on casting vertically downwards. This technique has a number of disadvantages such as control of metal head and metal constraint. The project intends to cast horizontally which alleviates these problems. (Funded by EPSRC and Kvaener Metals)

Rapid spray formed tooling

T. Rayment, P. Jones, Dr. Z. Djuric, Dr. S. Hoile, 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.)

Coupled eutectic growth in twin roll cast aluminium alloys

*T. Cockfield, Dr. M. Yun, Professor J.D. Hunt, Dr. K.M. Gatenby**

A range of aluminium alloys of eutectic composition are to be twin roll cast to investigate the extent of the coupled eutectic growth region. Alloys of this type are of interest because the large amount of eutectic can possibly improve the recrystallisation behaviour and therefore the mechanical properties of the twin cast roll sheet. (*Alcan International) (Funded by EPSRC and Alcan International)

The grain refinement of twin roll cast aluminium alloys

Dr. M. Yun, Professor J.D. Hunt

Grain refiners are traditionally added to aid casting and improve the castability of aluminium alloys. This project is investigating the relative efficiency of different grain refiner additions i.e. TiB₂, TiC, during the twin roll casting of commercial aluminium alloys. (Funded by EPSRC and London and Scandinavian Metallurgical Co. Ltd.)

Twin roll casting of superplastic SPZ Zn-Al

*Dr. M. Yun, Professor J.D. Hunt, T. Rance**

This material is traditionally ingot cast prior to a complex thermomechanical processing route which produces the very fine grain size necessary for superplasticity. Twin roll cast Zn-22wt%Al has been produced which exhibits superplasticity in the as-cast condition. Trials are underway to maximise this effect by investigating both the casting conditions and possible heat treatments. (*Custom Metalforms Ltd.)(Funded EPSRC and Custom Metalforms Ltd.)

Second generation Ti MMCs

Dr. K.H. Baik, Dr. H. Peng, Dr. P.S. Grant, Dr. F. Dunne, Professor B. Cantor*

New Ti alloy fibre reinforced MMC formulations are being manufactured by plasma spraying, sputter coating and hot uniaxial and isostatic pressing, and being assessed by detailed microstructural examination and residual stress characterisation (*Department of Engineering Science)(Funded by EPSRC, Rolls-Royce plc and QinetiQ).

Spray formed Ni alloys

A. Lambourne, M.K. Hedges, 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 EPSRC, Rolls-Royce and Allvac)

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)

Novel manufacturing routes for Al products

C.D.J. Manson-Whitton, Dr. P. Schumacher, 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.)

Improved processing of wrought Al alloys by modelling and control of grain refinement

Dr. P. Cizek, Dr. K.A.Q. O'Reilly, Dr. P. Schumacher, Dr. A.L. Greer*, Dr. R. Hamerton**, D. Bristow***

The performance of Al-Ti-C grain refiners in wrought Al alloys is being characterised to understand the nucleation mechanism and to develop quantitative modelling of the refiner action capable of application to a range of alloys and processing conditions. (*University of Cambridge; **Alcan International; ***London Scandinavian Metallurgical Company)(Funded by EPSRC, LSM and Alcan)

Continuous casting of copper base alloys

Dr. M. Yun, Professor J.D. Hunt, R. Bloomer*

The purpose of this project is to investigate the twin roll casting of copper based alloys and to compare the sheet with material produced by other continuous casting routes. (*Mason Precision Strip)(Funded by EPSRC and Mason Precision Strip)

Melt spun amorphous and nanocrystalline Al and Fe alloys

Dr. Y. Zhang, Dr. P.J. Warren, Dr. A. Cerezo, Professor B. Cantor

Amorphous and nanocrystalline Al and Fe alloys are being fabricated by melt spinning to form crystalline/quasicrystalline/amorphous composites for detailed TEM and FIM/AP investigations of microstructure. (Funded by EPSRC and in collaboration with Carpenter Technology and QinetiQ Farnborough)

Spray formed Al alloys

Dr. K-H. Baik, Dr. I.C. Stone, 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 the manufacture of Al-Li, Al-Zn-Mg and Al-Si alloys by spray forming and their downstream processing. At each process stage, the microstructure is investigated by SEM/TEM/EPMA and XRD, and microstructure related to final properties. (Funded by EPSRC and Joint Infrastructure Fund and in collaboration with Universities of Cranfield and Southampton, 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.

Manufacture and characterisation of nanostructured aluminium alloys

Dr. F. Prima, Dr. M. Tomut, Dr. I.C. Stone, Professor B. Cantor

Al-base nanocomposite materials containing high volume fractions of quasicrystalline dispersoids are being produced by rapid solidification and bulk processing techniques. The nanoscale microstructures formed during quenching are strongly dependant upon the thermal history of the melt due to cluster formation in the liquid. This project is part of an EU Research Training Network with 9 partners (www.materials.ox.ac.uk/nano-al)

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. (*University of Buenos Aires) (Funded by EU and British Embassy Korea S&T Fund)

Carbon fibre reinforced magnesium

*M. Russell-Stevens, Dr. K.A.Q. O'Reilly, Dr. P. Schumacher, P. Schultz**

Microstructural investigation of long fibre carbon fibre reinforced magnesium alloys manufactured by squeeze casting, as a function of casting parameters. (*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. P. Schumacher, 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)

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E. Phase Transformations, Surfaces and Interfaces

I - PHASE TRANSFORMATIONS

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

Dr. M.L. Jenkins, Professor J.M. Titchmarsh

Hardening due to formation of copper precipitates is a major problem for in-service performance of reactor-pressure-vessel steels. The project aims to answer 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?

Quantitative analysis of crystallisation processes in amorphous alloy films

G. Ruitenber, Dr. A.K. Petford-Long, Professor P.J. Dobson, R.C. Doole, Dr. C.N. Afonso***

In-situ TEM crystallisation experiments are being carried out on amorphous Sb-based alloy films with applications as ultra-fast phase-change optical storage media. The results are allowing quantitative data about the crystallisation kinetics to be obtained. The effects of the relaxation state of the amorphous structure on crystallisation kinetics are also being studied in both alloy and oxide films. (*Department of Engineering Science; **Institute of Optics, CSIC, Madrid, Spain) (Funded by EPSRC and Royal Society)

Structure and crystallisation kinetics of optical and magnetic nanocomposites

J-P. Barnes, N. Beer, Dr. 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)

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.

Nucleation kinetics of potent heterogeneous site

Dr. P. Schumacher

Heterogeneous nucleation of commercial grain refiner particles (TiB₂, TiC) is being studied as additions in amorphous Al alloys. Nucleation substrate surfaces are investigated in TEM and their properties measured in entrained droplet measurements. A kinetic adsorption model is being developed to predict quantitative nucleation rates. (Funded by EPSRC)

Experimental studies and modelling of cellular and dendritic growth

A. Chilton, Professor J.D. Hunt

The transition between cellular and dendritic growth is being studied experimentally and models will be developed to predict the transition. The models will be based on an existing axisymmetric cell/dendrite model. (Supported by Alcan International)

Modelling microstructure in multicomponent alloys

M. Shin, Professor J.D. Hunt

Diffusion based models are being used to predict microstructure in multicomponent alloys. The work extends an existing model which treats two components. The model predicts the path of the liquid, microsegregation, the non-equilibrium freezing range and treats three and four phase reactions. The programme uses the NPL MTDATA database to provide thermodynamic data. (Supported by Alcan International and in collaboration with NPL)

The development of a high temperature single pan scanning calorimeter.

Dr. H.B. Dong, Professor J.D. Hunt

A novel scanning calorimeter is being built to measure enthalpy up to temperatures of 1650 C. The heat flow within the calorimeter will be modelled numerically to improve the accuracy of the measurements. (Funded by EPSRC and in collaboration with NPL)

Modelling columnar and equiaxed growth

D.J. Browne, Professor J.D. Hunt

A three dimensional casting model is being developed to describe columnar and equiaxed growth.

Model alloys (ferritic steels), precipitation as a function of composition and ageing treatments using HREM techniques

Professor J.M. Titchmarsh, Dr. M.L. Jenkins, A.N Other

The embrittlement of pressure vessel steels is being investigated through a systematic investigation of the influence of alloying element content and heat treatment. High resolution imaging and microanalytical electron microscopy methods are used to identify precipitation and segregation in a series of model alloys. These results will be correlated with the variations in mechanical properties and related to models of toughness changes in neutron irradiated pressure vessel steels.

Scanning Calorimetry

T.O.R. Perry, Dr. H.B. Dong, Professor J.D. Hunt

In this work a calorimeter will be designed to give enthalpy as a function of temperature for large specimens (20-200g). The process will be modelled numerically to help process the data. It is hoped that this approach will give considerably increased accuracy and sensitivity.

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

*E.C. Kurum, Dr. H.B. Dong, Professor J.D. Hunt, Dr. H. Cama**

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)

Heterogeneous nucleation of Mg alloys

S. Srimanosaowapak, Dr. P. Schumacher

Heterogeneous nucleation of hex-Mg on carbide and boride particles is investigated in conventional casting experiments and in Mg-based glasses. Mg-based glasses allow the freezing-in of nucleation events during rapid cooling at the glass transition temperature. By this route the rapid growth of Mg from carbide and boride particles can be stopped and the nucleating particles identified and studied in detailed TEM investigations. These results are compared to conventional casting experiments where the efficacy of particles to promote fine grain sizes is studied.

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 500µm diameter and so, by comparison with other sampling techniques, the effect on the appearance of an object is minimal.

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.

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)

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)

III - SURFACE REACTIONS AND CATALYSIS

Controlled atmosphere analytical electron microscopy

R.C. Doole, Dr. J.L. Hutchison

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.

One-dimensional crystal growth inside single-wall carbon nanotubes

*Dr. J.L. Hutchison, Dr. J. Sloan, G. Brown, R. Carter, 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)

In-situ observation of solid-state reactions

Dr. J.L. Hutchison, Dr. M.J. Sayagues de Vega, Dr. F. Krumeich***

The controlled environment TEM is being used in a study of oxidation and reduction reactions of Nb, W and Mo. (*University of Seville; **ETH Zürich) (Funded by British Council and NATO)

Catalytic atom probe

P. Bagot, Professor G.D.W. Smith, Dr. A. Cerezo, T.J. Godfrey

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. (Funded by EPSRC and in collaboration with Johnson Matthey and Omicron Surface Science Ltd.)

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F. Characterisation

I - SCANNING TUNNELLING AND ATOMIC FORCE MICROSCOPY

Ultrasonic heterodyne force microscopy for studies of dynamics of nanoscale non-mechanical properties

*Dr. O.V. Kolosov, Dr. B.D. Huey, Professor G.A.D. Briggs, Professor O.B. Wright**

The physical principles, theoretical background and technical realization of the novel principle of mechanical heterodyne force microscopy is developed. This novel Scanned Probe Microscopy approach enables measurements and mapping of time-dependent physical properties of studied object (e.g. electrical, optical, thermal, etc.) with the nanometre scale spatial resolution and sub-nanosecond time sensitivity. (*Dept. of Applied Physics, Hokkaido University, Japan.) (Funded by the Japanese Society for Promotion of Science and British Council)

Investigation of the physics of dynamic tip-surface interaction at ultrasonic time-scale

Dr. B.D. Huey, Dr. O.V. Kolosov, Professor G.A.D. Briggs

Dynamic interactions between a tip and a sample surface are studied by performing ultrasonic, waveguide and heterodyne force microscopy experiments in different controlled environments. (Funded by EPSRC)

Semiconductor metallization in variable temperature STM/STS

Dr. M.R. Castell, Professor G.A.D. Briggs, Dr. C. Norenberg, Dr. M. Martin Fernandez

Technologically important refractory metals (Ti, Co, etc) will be deposited from UHV evaporators onto semiconductor surfaces in variable temperature STM. The crystallographic characteristics of the contacts will be investigated by STM, RHEED/LEED and AES, and the physical characteristics of the resulting barriers will be measured by STS.

Experimental development of heterodyne force microscopy

Dr. B.D. Huey, Dr. O.V. Kolosov, Professor G.A.D. Briggs

Implementation of Heterodyne Force Microscopy (HFM) is in progress. Experimental research seeks to determine the capabilities and limitations of the technique for the study of time-dependent processes on a nanometer scale and to realise the HFM potential for the time sensitivity on the sub-nanosecond time scale. (Funded by EPSRC)

Study of nanoscale material properties using ultrasonic-based scanning force microscopy techniques

Dr. B.D. Huey, Dr. O.V. Kolosov, Professor G.A.D. Briggs, Dr. H.E. Assender

Ultrasonic, waveguide and heterodyne force microscopy are used to investigate the nanoscale mechanical structure of materials of different origin, including semiconductor quantum dots, polymer composites and metallic compounds.

Nanoscale dynamics of ferroelectric domains

Dr. O. Kolosov, Dr. F. Rusanescu, Professor L. Eng***

The nanoscale structure of ferroelectric domains and the dynamics of domain switching are studied using scanning probe microscopy. (*Istituto di Acustica, Rome, Italy; **Technical University of Dresden, Germany)

Direct measurement of interatomic potentials

Professor J.B. Pethica, L. Giberti, Dr. S.P. Jarvis**, Dr. H. Tokumoto***

A new AFM allows the direct mechanical measurement of short range interaction potentials between tip and surface. Strong interactions can be accessed without mechanical instability. (*Trinity College, Dublin; **JRCAT, Tsukuba, Japan) (Funded by EPSRC and Paul Instrument Fund)

Atomic resolution AFM*L. Giberti, Professor J.B. Pethica**

A new AFM designed and built in-house, gives real space surface atomic resolution of forces and force gradients, using sub-Å oscillation amplitudes. It is shown that atomic resolution is correlated with dominance of short range interactions. (*Trinity College, Dublin) (Funded by EPSRC and Paul Instrument Fund)

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)

Forces on single atoms in STM*Professor J.B. Pethica*, L. Giberti, Dr. J. Nieminen***

STM images change with tip-surface separation as a result of forces present. Experiment and MD modelling are combined to determine forces at individual atoms. Metals and halogen adsorbates are presently studied. (*Trinity College, Dublin; **University of Tampere, Finland)

Room temperature manipulation of surface atoms*Professor J.B. Pethica*, Dr. R.G. Egdell***

Individual bromine atoms can be placed at specified sites on a copper surface and nanostructures written at room temperature. The mechanisms of atomic manipulation and their possible specificity are under investigation. The study is being extended to variable temperature. (*Trinity College, Dublin; **Inorganic Chemistry Laboratory)

STM & AFM of metals on oxides at variable temperature*Professor J.B. Pethica*, Dr. C.E.J. Mitchell**, Dr. R.G. Egdell**, Professor J.S. Foord****

A new variable temperature STM and XPS system is used to study catalytic oxides and metal islands thereon. Surfaces under investigation include SnO₂, WO_n and tungsten bronzes, ZnO. (*Trinity College, Dublin; **Inorganic Chemistry Laboratory; ***Physical Chemistry Laboratory) (Funded by EPSRC)

Growth and characterization of quantum silicide and nitride islands*Professor G.A.D. Briggs, Dr. M.R. Castell, Dr. S.D. Kenny, Dr. C. Norenberg, Dr. M. Martin Fernandez, R. Oliver, Professor A.P. Sutton*

The growth and properties of silicide and nitride islands 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 study both metallic and semiconducting islands. 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.

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)

Nanostructures on the SrTiO₃ (001) Surface*Dr. M.R. Castell*

Atomically resolved scanning tunneling 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 cubic SrO on a TiO₂ terminated surface containing ordered TiO₂ defects. Further characterization and metal island growth on these surfaces is currently being carried out. (Funded by The Royal Society)

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)

Ferroelectric domain characterization

Dr. B.D. Huey, Dr. O.V. Kolosov, Professor G.A.D. Briggs

Ultrasonic force microscopy, electrostatic force microscopy, and piezoresponse imaging are applied to investigate the piezoelectric characteristics of individual domains in ferroelectric thin films. Using this combination of techniques, domain switching can be directly measured at frequencies ranging from Hz to 100 MHz. (Funded by US-NSF and Marshall Aid Commission)

Ultrasonic Force Microscopy characterization of Focused Ion Beam implantation and damage

Dr. B.D. Huey, Dr. R. Langford

The spatial extent of Gallium ion implantation and/or damage from FIB is measured using UFM. This allows characterization of the FIB system, in particular to identify proper implantation parameters for a given damage threshold. UFM sensitivity and resolution are also investigated using the wide variety of implantation profiles available with the FIB.

II - FIELD-ION MICROSCOPY AND ATOM PROBE MICROANALYSIS

Atom probe microanalysis techniques

Dr. A. Cerezo, T.J. Godfrey, P. Bagot, 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 $m/Dm=600$ 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 JREI and in collaboration with Oxford Nanoscience Ltd., Omicron Surface Science Ltd. and Johnson Matthey plc.)

Scanning atom probe

T.J. Godfrey, O. Dimond, Dr. 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. (*Omicron GmbH) (Funded by BRITE/EURAM and in collaboration with Omicron GmbH, Oxford Nanoscience Ltd. and Seagate Ltd.)

Atom probe studies of 2xxx Al alloys

L. Davin, Dr. 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, Imperial College.) (Funded by EPSRC, Airbus and QinetiQ)

Early stages of precipitation in 7xxx series aluminium alloys

*Dr. G. Sha, Dr. 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) (Funded by EPSRC, in collaboration with Alcoa)

3D Reconstruction of atom probe data

O. Dimond, Dr. P.J. Warren, Dr. 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. (*Omicron GmbH)(Funded by Oxford Nanosciences Ltd. and Omicron GmbH)

Atom probe analysis of information storage materials

Dr. Y.Q. Ma, Dr. A. Cerezo, Dr. 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)

Early stages of precipitation in 6XXX automotive sheet

D. Vaumousse, Dr. 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. (Funded by EPSRC and Alcan International)

Thermal ageing of steels

Dr. S. Hirose, Dr. 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 Power Engineering)

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

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

High resolution electron microscopy (HREM)

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

Analytical electron microscopy (AEM)

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

High resolution analytical electron microscopy

A JEOL 2010 high resolution electron microscope has been installed in 1994. This instrument 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 equipped with a comprehensive range of advanced analytical facilities, including light-element sensitivity EDX, parallel electron energy loss spectroscopy (PEELS), energy-filtered imaging (GIF), an electrostatic biprism for electron holography, a high performance CCD camera and a piezoelectric, drift correcting specimen stage. With a capability of microanalysis and electron diffraction from areas down to <0.4nm in diameter, and a spatial resolution of 0.16nm, this instrument is being used in a wide range of applications, involving new nanostructured materials.

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 (<1x10⁻¹⁰mbar). 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 LaB₆ 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.

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 recently installed 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.

Nanometer scale induced structure between amorphous layers and crystalline materials

Professor D.J.H. Cockayne, Professor A.P. Sutton, Dr. G. Möbus, 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.

Polyhedral and cylindrical metal chalcogenides

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

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

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)

In-situ TEM studies of magnetic domain structure

Dr. 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)

Disorder in complex oxides

*Dr. J.L. Hutchison, Dr. J. Sloan, Dr. M.-J. Sayagues de Vega**

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. (*University of Seville) (Funded by British Council and NATO)

The structure of copper precipitates in age-hardening steels

Dr. M.L. Jenkins, Professor J.M. Titchmarsh

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.

Behaviour of carbon in controlled environment electron microscopy

*Dr. J.L. Hutchison, Dr. A.P. Burden**

The behaviour of various forms of carbon in the gas-reaction cell is being investigated. The interaction of the electron beam with the volume of gas above the specimen produces a plasma which in turn generates new structures - including fullerenes. The effects of different gases and other parameters are being studied with a view to understanding the mechanisms of fullerene growth. (*Rutherford Appleton Laboratory)

Integrated quantitative HREM analysis and molecular modelling

Dr. G. Möbus

A program package for numerical structure retrieval from HREM images, using iterative simulation and digital image matching, is extended and maintained with respect to: (i) improving user-friendliness and conversion to a public-domain product; (ii) including three-dimensional structural coordinates in extension to projected atomic column positions to refine 3D atomic structures; (iii) a methodology is developed which allows interface and dislocation structure models to be characterised simultaneously by an energy value (from semi-empirical potentials) and by an experimental R-factor (from matching simulated to experimental HREM-images). (Funded by EPSRC)

Determination of gradual partial coherence of hetero-interfaces using quantitative HREM

*Dr. G. Möbus, Dr. B.J. Inkson, Dr. M. Hytch***, Dr. A. Trampert**, Dr. T. Wagner**

High-resolution electron micrographs of a large variety of hetero-interfaces (metal-metal, metal-ceramic, semiconductors) are digitally analysed. A novel combination technique measures local amplitude and phase spectrum of lattice fringes with high spatial resolution. Presence of strain and misfit dislocations are detected as a function of interface distance. A classification scheme for hetero-interfaces is developed from the measurements. (*Max-Planck-Institut fuer Metallforschung, Stuttgart, Germany,**Paul Drude Institut, Berlin, Germany; ***CNRS, Paris-Vitry, France)

Atomic-Resolution EELS/ELNES: Impact of Cs-correction and beam propagation

*Dr. G. Möbus, Dr. C.J.D. Hetherington, Dr. S. Nufer**

Optimum conditions of beam formation for nanoanalysis and STEM imaging will be examined around a newly developed software package for dynamical propagation of subnano-beams. The project comprises: (i) Tests of nanobeam formation and beam propagation in materials on the JEM 3000F, including matching of simulated to experimental data. (ii) prediction of future modes of imaging and analysis in STEM with and without Cs-correction; (iii) Evaluation algorithms for "single atomic column" EELS/ELNES/EDXS at grain boundaries. (*MPI fuer Metallforschung, Stuttgart, Germany)

CBED analysis of strain fields in nanocomposites with highest spatial resolution

Dr. G. Möbus

Convergent beam electron diffraction is applied using the highly focused beam of the FEGTEM JEM-3000F to obtain local information on strain distributions within nanocomposite materials. An automated beam propagation mode to scan two-dimensional areas of interest on the specimen will be implemented.

Quantitative ADF Imaging of Nanocomposite Materials

Dr. G. Möbus, Dr. M. Ceh, S. Sturm*, Dr. A. Rechnik*, Dr. B.J. Inkson, Dr. T. Wagner***

The imaging properties of ADF and HAADF imaging in a JEM-2010F FEGSTEM are studied with respect to a correct interpretation of the Z-dependency of the projected integrated contrast in nanoscale composite materials. Examples comprise buried nanoparticles in metallic matrix and metallic multilayers (*Jozef-Stefan-Institute, Ljubljana, Slovenia; **MPI fuer Metallforschung Stuttgart, Germany)

3D microstructural characterisation of deformed nanostructures using FIB

Dr. B.J. Inkson, T. Steer, Dr. M. Bobji, Dr. G. Möbus, Dr. O. Kraft, Dr. T. Wagner**

A new technique of characterising nanostructures in 3D by serial FIB sectioning and 3D computer reconstruction is being developed. 3D microstructural maps of deformation under indents, grain shape around deformation sites and crack profiles are being determined and related to the local mechanical properties determined by nanotesting (Funded by the Royal Society, EPSRC, DAAD and The British Council) (*MPI fuer Metallforschung, Germany).

Development of Spectroscopic Tomography for 3D Composition Mapping of Nanomaterials.

Dr. G. Möbus, Dr. B.J. Inkson, Professor J. Titchmarsh, Professor D.J.H. Cockayne, Dr. S.H. Kim, Dr. R. Langford, R.C. Doole

Energy filtered transmission electron microscopy (EFTEM) and EDXS-mapping are used to obtain compositional maps over very large ranges of angular tilt. Tomographic reconstruction and display algorithms are developed to account for the specific properties of EELS and EDXS based data sets. Specimen preparation techniques are optimised towards high tilt capabilities. Applications comprise nanoparticles, nanocomposites, multilayered metal and semiconductor structures.

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*, Professor B. Cantor*

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 JREL)

Development of transmission electron microscopy for studies of crack tips

Professor J.M. Titchmarsh, Dr. Y. Huang, I Armonson, N Peat**

Environmentally Assisted Cracking and Irradiation Assisted Stress Corrosion Cracking are phenomena which occur in power generating plant and are difficult to predict or control. The influence of microstructure and chemistry on crack growth is being investigated by developing the techniques to prepare TEM specimens containing crack tips and characterising microstructures. Correlation between crack tip microstructure and environmental parameters will be made. (*Rolls Royce Marine Power)

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, C. Ward, Dr. W. McBride, Dr. D. Nguyen Manh, Professor D. McKenzie**

The structure of amorphous thin films and small volumes of amorphous materials is being investigated using energy selected electron diffraction combined with atomistic modelling. Refinement procedures are being developed which will allow differentiation between alternative structural models. (*University of Sydney)

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. G.M. Möbus, 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 will include a field-emission-gun, 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.

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

Dr. J.L. Hutchison, Dr. J. Sloan, Dr. A.I. Kirkland, Dr. W.O. Saxton**

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. (*University of Cambridge) (Funded by EPSRC)

Quantum dot and quantum well structures

Professor D.J.H. Cockayne, Professor G.A.D. Briggs, C. Lang, Dr. J. Zou, Dr. L. Xiaozhou*, Professor R. Nicholas**, Dr. C. Marsh*

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. (*University of Sydney; **Department of Physics)

3-D microstructural analysis using a FIB system

Dr. R.M. Langford, Professor J.M. Titchmarsh, Dr. B.J. Inkson, Dr. G. Möbus, T. Steer

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)

Preparation of TEM specimens for high resolution electron microscopy

Dr. R.M. Langford, Dr. Y. Huang, S. Lozano-Perez, Dr. A.K. Petford-Long

Techniques are being developed to prepare site-specific TEM cross-section and plan-view specimens. In particular, the effect of different milling parameters and methods to manipulate the specimens in-situ for broad-beam ion milling are being investigated.

Development of an advanced FIB system for micromachining applications

Dr. R.M. Langford, Dr. 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)

Diffuse and inelastic scattering in RHEED

Dr. S.L. Dudarev*, Professor L.-M. Peng**, Dr. Z. Mitura***, Professor M.J. Whelan

Methods are being developed in order to understand diffuse scattering from rough crystal surfaces and investigate the effect of inelastic scattering on RHEED intensity. (*UKAEA Fusion, Culham Science Centre; **Chinese Academy of Science; ***University of Krakov, Poland)

TEM investigation of stress corrosion cracking in Inconel 600

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)

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

Dr. R.M. Langford, Dr. Y.Q. Ma, Dr. A.K. Petford-Long, Dr. 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)

Characterisation of RHEED oscillations

Dr. Z. Mitura*, Dr. S.L. Dudarev**, Professor M.J. Whelan, Professor L.-M. Peng***

The phenomenon of reflection high energy electron diffraction oscillations is being investigated theoretically. Special attention is being paid to the phase of oscillations as this quantity may be both precisely measured experimentally and determined computationally. (*University of Krakov, Poland; **UKAEA Fusion, Culham Science Centre; ***Chinese Academy of Science)

IV - NUCLEAR MICROSCOPY WITH THE SCANNING PROTON MICROPROBE

The Scanning Proton Microprobe (SPM) was established in its present form in the Nuclear and Astrophysics Laboratory in 1988 following several years of development in the then Nuclear Physics Department, and became a part of the Materials Department in 1997. The instrument uses a focused beam of 1 - 3 MeV protons (or alpha particles or oxygen ions as required) to carry out elemental microanalysis and mapping. At present the facility uses the techniques of *proton-induced x-ray emission* (PIXE) and *Rutherford backscattering* (RBS) to obtain elemental compositions over the whole periodic table with a detection limit in the range of 1 - 100ppm

and a spatial resolution of $1\mu\text{m}$. RBS also has the possibility of determining depth profiles or surface film thickness in suitable samples. In addition to these main techniques, other interactions are exploited for more specialised applications. These include *ion beam induced charge* (IBIC) for mapping the active regions of semiconductor devices, *elastic recoil detection analysis* (ERDA) for measuring near surface ($<500\text{nm}$) depth profiles of light elements (H, D, He etc.), *total reflection PIXE* (TRPIXE) for measuring metal concentrations in surface monolayers and *scanning transmission ion microscopy* (STIM) for mapping the thickness/density variations in thin ($<30\mu\text{m}$) samples. In crystalline materials most of these interactions can be used in conjunction with channelling to investigate lattice properties and defects.

The high energy ions are produced by a small tandem Van de Graaf accelerator and the beam is either focused to a $1\mu\text{m}$ diameter spot in a high vacuum target chamber (using a novel high precision quadrupole triplet lens) or brought into air through a thin foil to allow analysis at $250\mu\text{m}$ resolution of large objects or objects incompatible with vacuum. A programme of instrumentation development aimed at enhancing the capability of the technique and producing a beam of $0.1\mu\text{m}$ diameter is running in parallel with collaborations in wide range of analytical projects.

Metal uptake by hyperaccumulating plants

Professor J.A.C. Smith, Dr. G.W. Grime*

Certain plants native to metal rich soils have the ability to sequester high levels of metals in their tissues, and these are being investigated with a view to their use in bio-remediation of polluted soils. MicroPIXE is being used in a study of the transport mechanism and storage sites of metals in a range of plants known to be hyperaccumulators. In the nickel hyperaccumulating plant *Alyssum lesbiacum* it was found that the nickel is stored in modified leaf hairs on the leaf surface. (*University of Oxford Department of Plant Sciences) (Funded by NERC)

Determination of hydrogen and metals on mineral surfaces

Dr. R.A. Wogelius, Dr. G.W. Grime*

The SPM has been used in two studies of chemical interactions on mineral surfaces. 1) ERDA using a beam of 7.5MeV O^{16} ions has been used to investigate the depth distribution of hydrogen on clean mineral crystal surfaces hydrated under high temperature and pressure. 2) Total reflection PIXE (using a beam at glancing incidence) has been used to determine the concentration of metals reacted onto the surface of mineral crystals at sub-monolayer concentrations. This is presently being used to determine the surface uptake of oil well scale inhibitors on typical oil well minerals. (*Department of Earth Sciences, University of Manchester) (EPRSC funded consortium)

Development of a 0.1 micron Scanning Proton Microprobe beamline

Dr. G.W. Grime

A new beamline is under development which is planned to have a beam diameter of 0.1micron with sufficient beam current to carry out PIXE, RBS and STIM analysis. The increased resolution will be achieved with a combination of a new design of high demagnification magnetic quadrupole triplet lens and careful engineering to ensure that the system is mechanically and electrically stable to the high tolerances required. The expected beam current at 0.1micron beam resolution is 30pA of 3MeV protons. At the very low beam currents required for STIM and IBIC the beam diameter is predicted to be $10 - 30\text{nm}$. (Funded by the Wellcome Trust)

Reference materials and standardisation techniques for trace element micro-analysis

Dr. G.W. Grime with a consortium of EU laboratories (Coordinator Prof. F. Adams)*

Well characterised reference materials are essential for quantitative chemical analysis. Normal reference materials usually have a grain structure which makes them unsuitable for microbeam techniques (e.g. electron probe, x-ray fluorescence microprobe, nuclear microprobe). In this EC funded project a consortium of six EU laboratories including the Community Bureau of Reference Materials are developing trace element standards based on ion implanted glasses with no detectable microstructure. The laboratories combine expertise in all forms of probe microanalysis. In Oxford we are also developing the combination of Rutherford Backscattering analysis and proton induced x-ray emission analysis as a standardless trace element technique. (*University of Antwerp)

V - RADIATION DAMAGE

Displacement cascade processes

Dr. M.L. Jenkins, Dr. M.A. Kirk, Dr. C. Abromeit**,
Dr. H. Fukushima****

Displacement cascade processes in various materials are being studied by diffraction-contrast, high-resolution and analytical electron microscopy techniques. The "disordered zone" technique is being used to study cascades in the ordered alloys Ni₃Al and Cu₃Au. Studies are also being extended to high-Tc superconductors and to intermetallics. Some of the work involves in-situ heavy-ion irradiations in the Argonne IVEM-Tandem Facility. (*Argonne National Laboratory; **Hahn Meitner Institut, Berlin; ***Hiroshima University) (Funded by British Council and U.S. D.O.E.)

Investigations of the stability of precipitates under cascade-producing irradiation

Dr. M.L. Jenkins, Professor G.D.W. Smith, Professor J.M. Titchmarsh

The stability of various precipitate phases in copper, nickel and iron matrices under heavy-ion irradiation is being investigated using high-resolution electron microscopy (in collaboration with the Hahn-Meitner Institute, Berlin) (Funded by EPSRC)

Mechanisms of embrittlement in reactor pressure vessel steels

*Dr. M.L. Jenkins, Professor J.M. Titchmarsh,
Professor Sir Peter Hirsch, Dr. M.A. Kirk**

Electron microscopy of heat - treated and irradiated pressure vessel steels and model alloys is being carried out to identify the mechanisms by which these materials become embrittled during neutron irradiation, with particular emphasis on (i)the precipitation of copper-rich particles, and (ii)identification of the matrix component of hardening.(*Argonne National Laboratory, Argonne IL, USA)

Quantum Electron Microscope Imaging of Nanoclusters under Weak-Beam Conditions

Dr. M.L. Jenkins, Dr. S.L. Dudarev, Professor A.P. Sutton, Professor J.M. Titchmarsh, Z. Zhou ,
Professor C.B. Carter**, 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 further development of a computer code implementing the original Howie and Basinski equations written at the University of Minnesota by the group led by Professor C B Carter, 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 Fusion Association; **University of Minnesota; ***Argonne National Laboratory)

Inelastic scattering in weak-beam images and its implications for quantitative contrast measurements in the transmission electron microscope.

*Dr. M.L. Jenkins , S.P. Martin, Dr. M.A. Kirk
(Argonne National Laboratory)*

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 determining more precisely the contributions to images of inelastically scattered electrons. Questions to be addressed include: How useful is energy-filtering in improving the quality of weak-beam images? Is energy filtering essential if experimental weak-beam images are to be compared with simulated images quantitatively?

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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 houses a suite of Hewlett-Packard and Silicon Graphics workstations which have sole access to a very powerful HP Exemplar S-class computer. 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. In particular, the Exemplar S-class computer was bought with matching funds from Hewlett-Packard's Convex Division, Information Storage Group, and Corporate Laboratories. The Silicon Graphics Power Challenge was bought with funds from BNFL.

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

Professor D.G. Pettifor, Dr. D. Nguyen Manh, Dr. D. 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). (*University of Surrey; **University of Pennsylvania) (Funded by EPSRC).

Studies of amorphous carbon films by electron diffraction and modelling

*Professor D.J. H. Cockayne, Dr. W. McBride, Dr. D. Nguyen Manh, Dr. S. Mukhopadhyay, Professor D.G. Pettifor, Professor D.R. McKenzie**

Analytic bond-order potentials (BOPs) are being developed and applied to modelling the growth of amorphous carbon films for comparison with in-house electron diffraction and EELS measurements on films grown at the University of Sydney. (*University of Sydney) (Supported by British Council Collaborative Research Project)

Modelling the magnetoresistive behaviour of spin-valve devices

Professor D.G. Pettifor, Dr. E. Tsymbal, Dr. A.K. Petford-Long, Dr. J.A. Brug, Dr. T.C. Anthony*, Dr. C. Moorhouse**

The magnetoresistive behaviour of metallic and tunnelling spin valve structures and devices is being modelled within a Tight Binding description of the electronic structure. The theoretical insights and predictions are correlated closely with the experimental programme both at HP Laboratories and Oxford. (*HP Laboratories, Palo Alto) (Funded by HP Laboratories)

Modelling diffusional phase transformations in the presence of elastic interactions

Professor A.P. Sutton, Dr. A. Cerezo, D. Mason

Earlier work has shown the necessity of using a vacancy mechanism of diffusion to model diffusional phase transformations in metallic alloys that occur on the 1-10 nanometre scale. Only when the correct mechanism of diffusion is used at the atomic scale will morphologies, kinetics and mechanisms of growth and coarsening be described correctly. In this work elastic interactions are being introduced to model transformations in alloys containing misfitting atoms. The elastic interactions are described by lattice Green's function methods we are developing. (Funded by EPSRC)

Simulations of the electronic and atomic structures of oxide surfaces

Dr. S.L. Dudarev, Professor A.P. Sutton, Professor G.A.D. Briggs, Dr. D.T. Goddard***

A new simulation programme is being applied to model surface reconstructions of oxide surfaces, to assist the interpretation of STM images. The oxides display strong electron correlations, e.g. NiO and UO₂, and they are representative of a large class of materials that display important catalytic properties. (*UKAEA Fusion, Culham Science Centre; **Research and Development, BNFL Springfield) (Funded by BNFL)

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)

Dynamical Ising model simulations of phase separation

Dr. S. Hirose, Dr. G. Sha, Dr. 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 EPSRC and Rolls Royce Power Engineering)

Mapping of magnetisation distributions in thin layered films

Dr. A.K. Petford-Long, Dr. B. Warot

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, Dr. S.G. Roberts

We are developing models 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.

First Principles tight binding package for general applications

Dr. S.D. Kenny, Professor A.P. Sutton, Dr. A.P. Horsfield***

A multi-application, first principles, LCAO density functional program is being developed for use inside the Materials Modelling Laboratory. (*Department of Mathematics, Loughborough University; **Fujitsu European Centre for Information Technology)(Funded by Fujitsu)

Modelling adhesion between polymers and inorganic substrates

Dr. T.R. Walsh, Professor A.P. Sutton

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. (Funded by Hewlett-Packard in collaboration with Virginia Polytechnic Institute and University of Massachusetts)

Carbon-based nanostructures

Professor E.G. Wang, Professor Lianmao Peng*, Dr. Gang Lui*, Dr. D. Nguyen Manh, Professor D.G. Pettifor*

The structure, of carbon-based nanostructures will be predicted using analytic bond-order potentials and compared with electron microscope images. (*Centre for Condensed Matter Physics, Beijing, China) (Funded by Royal Society -CAS joint research project)

First principle studies of transition metal sulphides

H.M. Sithole, P.S. Ntaohae*, H.R. Chauke*, Professor P.E. Ngoepe*, Dr. D. Nguyen Manh, Professor D.G. Pettifor*

The electronic structure, equation of state and structural properties of iron and noble metal sulphides are being predicted using first principles density functional theory. (*Materials Modelling Centre, University of the North, South Africa) (Funded by Royal Society - FRD collaborative project)

Modelling of growth of aerosol metal oxide nanoparticles

*Professor A.P. Sutton, P.J.D. Campbell, Dr. D.T. Goddard**

A new approach is being developed to the mathematical description of growth of metal oxide nanoparticles. The purpose of the study is to understand how the distribution of nanoparticles in their size and shape evolves in time and how the nature of this evolution depends on the process conditions. (*Research and Development, BNFL Springfield) (Funded by EPSRC and BNFL)

Atomistic and microscopy simulations for three-dimensional misfit-dislocation networks of heterointerfaces

A. Levay*, Dr. G. Möbus, Professor G. Tichy*, Professor V. Vitek**

Molecular statics relaxations of metallic thin films on rigid substrates are combined to multislice simulations of high-resolution electron microscopy. The aim is to examine the visibility of the misfit dislocation networks in various directions of projection and to decide about real structural features and electron diffraction artefacts. The first model system comprises hexagonal and trigonal networks in Nb thin films. (*Eötvös University, Budapest, Hungary; **University of Pennsylvania, USA)

Modelling secondary electron emission from surfaces with inequivalent terminations

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

Objects with more than 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, Professor G.A.D. Briggs, Dr. Y. Tsukuhara*

A new Monte Carlo technique has been developed and applied to the growth of SiO_x 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. (Funded by *The Toppan Printing Co.)

Modeling the evolution of cascades in fusion reactor materials

Professor A.P. Sutton, T. 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 failure 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 microcrack-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)

MBE growth of spintronic materials

Professor D.G. Pettifor, Dr. I. Oleinik, 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).

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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 6×10^3 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.

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)

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.

A study of Byzantine copper alloy metalwork

*Dr. J.P. Northover, Dr. M. Saghie 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)

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).

Copper extraction at Ross Island, Co.Kerry.

*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)

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

Anglo-Saxon Ferrous Technology

C.J. Salter, G. Hey*, Dr. B.J.J. Gilmour, K. Penn**, T. Mallin***

A systematic survey of the ferrous artefacts from a number of East Anglian and Midland sites is being carried out to determine range and distribution of various Anglo-Saxon black-smithing skills and technologies. (*Oxford Archaeological Unit; **Norfolk Archaeological Unit; ***Cambridgeshire Archaeology)

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 Archeology)

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

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, Universität Zürich, Switzerland; **Institut für Ur-und Frühgeschichte, Universität Wien, Austria)

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.

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 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)

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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