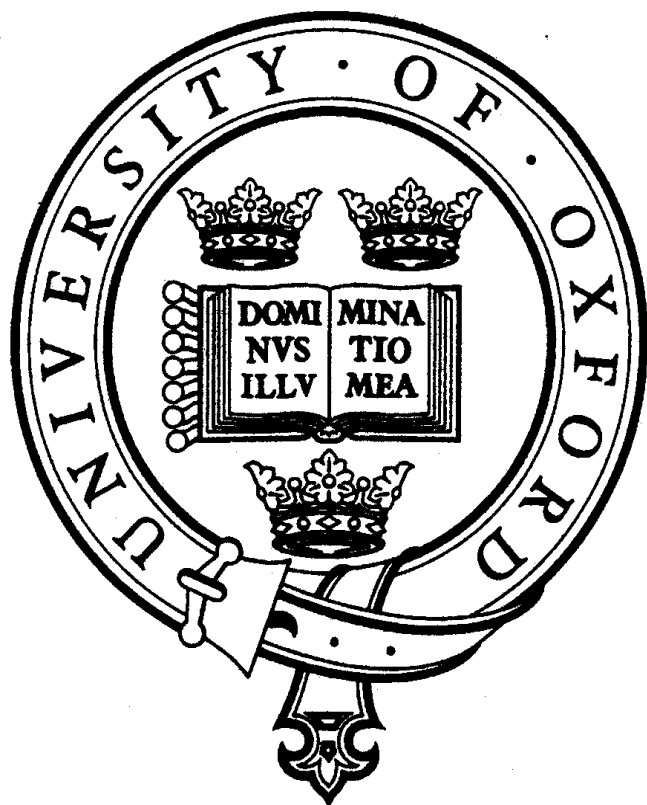


Department of Materials

University of Oxford

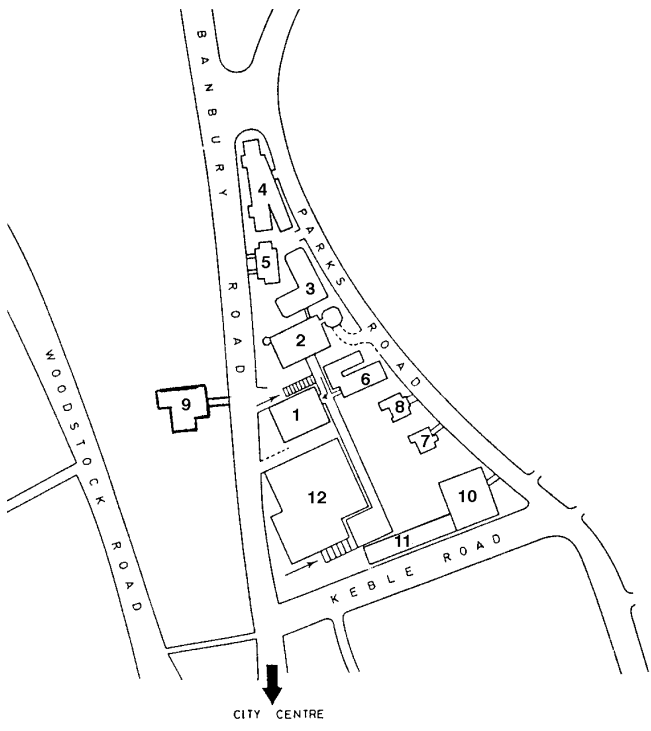
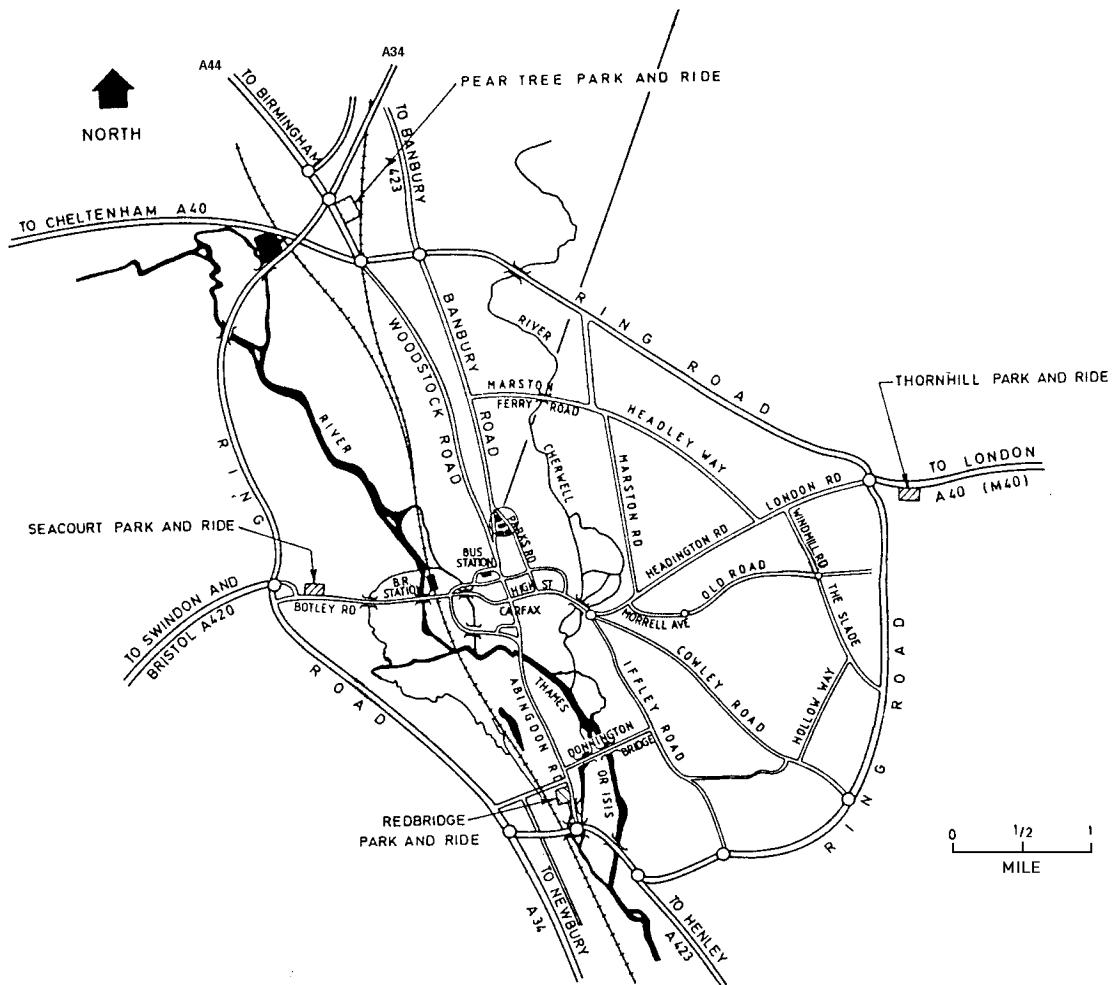


Research in Progress

1999-2000

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21 Banbury Road (9)

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Foreword from the Head of Department

The objectives of the Department of Materials at Oxford University 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 two years include:

- 1 2 new Professorships, in electron microscopy (David Cockayne) and structural integrity (John Titchmarsh);
- 2 4 elections to Fellowships of the Royal Society (David Cockayne and John Pethica) and the Royal Academy of Engineering (Richard Brook and myself);
- 3 6 promotions to personal professorships (Adrian Sutton and Andrew Briggs) and readerships (Chris Grovenor, John Hutchison, Amanda Petford-Long and John Sykes);
- 4 almost 100% increase in the Department's research income;
- 5 over £8m from the Joint Infrastructure Fund, to purchase cutting edge equipment for atomically engineered, nanoscale materials processing and analysis; and
- 6 the launch of the new £22m Begbroke site, which doubles the Department's space, and sets up a unique combination of industry-linked materials research and spin-out science park.

The Department was founded by Professor Hume-Rothery in 1956. At present, it consists of about 30 academics and senior researchers, 30 technicians and secretaries, 50 postdoctoral researchers and visitors, 100 research students and 120 undergraduates. The Department is part of an integrated Faculty of 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.

Materials teaching and research is increasingly important world-wide for economic prosperity. Per capita income and export earnings for a country are correlated with the size of its manufacturing industry, and the development and application of materials is a key enabling technology, as demonstrated by the government's Technology Foresight exercise. Industry depends critically on graduate employment and on innovations developed in collaboration with universities. The Department is developing strategic industrial alliances to meet industry's R&D, employment and continuing education needs.

The nature of advanced materials such as superconducting ceramics and metal/ceramic composites makes it difficult to draw sharp dividing lines between the traditional categories of metals, ceramics and polymers. Materials engineering is holistic, with complex materials architecture being used to achieve specific properties in a component or device, e.g. the metal interconnect/insulator/semiconductor structure in a microelectronic circuit, or the thermal barrier/compliance bond coat/aluminised corrosion resistant layer on a superalloy aeroengine component. The Department's research is organised, therefore, around three areas of expertise, processing, modelling and characterisation, for application across the whole range of materials problems.

The Oxford Centre for Advanced Materials and Composites (OCAMAC) co-ordinates industrial materials research across the Faculty of Physical Sciences. The new Director of OCAMAC is Patrick Grant. We have appointed seven new lecturers, are building a series of new laboratories and are commissioning pilot scale manufacturing facilities, to enhance our long-standing strengths in metallurgical, ceramic and microelectronic processing, and to promote recent initiatives in polymer and biomedical materials processing. The Materials Modelling Laboratory (MML) is based on the concept of linking models at the electronic, atomistic, microstructural and macroscopic length scales. The Director of the MML is David Pettifor. We have recently installed new computer facilities in what is the largest materials modelling laboratory in the UK, and we have just appointed two further new lecturers in the modelling field. Characterisation is the Department's traditional strength, with a unique combination of expertise and facilities in electron, field-ion, atom probe, acoustic, scanning tunnelling, atomic force and scanning proton microscopy. We have just installed the first 300kV field emission gun transmission electron microscope (FEGTEM) in Europe, and have secured funding for next generation transmission electron microscope, nanoscale secondary ion mass spectroscopy, 3D atom probe and scanning tunnelling/atom force microscope equipment. We have appointed three new professors and lecturers in materials characterisation fields.

This booklet describes the full range of 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 1999

Professor B. Cantor
Head of Department

Professors

Professor B. Cantor, FREng

*Cookson Professor of Materials
Head of Department*

Professor D.G. Pettifor, FRS

*Isaac Wolfson Professor of Metallurgy
Director of the Materials Modelling Laboratory*

Professor D.J.H. Cockayne, FRS

Professor in Physical Examination of Materials

Professor J.M. Titchmarsh

*The Royal Academy of Engineering/ AEAT / INSS
Research Professor in Microanalysis and Structural Integrity*

Professor C.C. Bradley

Visiting Professor

Professor G.A.D. Briggs

Professor of Materials

Professor R.J. Brook, OBE, FREng

Professor of Materials

Professor J.W. Christian, FRS *

Emeritus Professor

Professor B.L. Eyre, FREng

Visiting Professor

Professor Sir Peter Hirsch, FRS *

Emeritus Professor

Professor J.D. Hunt

Professor of Materials

Professor J.B. Pethica, FRS

Professor of Materials

Professor G.D.W. Smith, FRS

Professor of Materials

Professor A.P. Sutton

Professor of Materials

Professor M.J. Whelan, FRS *

Emeritus Professor

Readers

Dr. J.L. Hutchison

Director of Graduate Studies

Dr. J.M. Sykes

Director of Undergraduate Studies

Dr. C.R.M. Grovenor

Dr A.K. Petford-Long

Lecturers

Dr. P.S. Grant

*Director of Oxford Centre for
Advanced Materials and Composites*

Dr. H.E. Assender

Dr. K.A.Q. O'Reilly

Dr. D.G. Bucknall

Dr. S.G. Roberts

Dr. A. Cerezo

Dr. R.E. Rudd

Dr. J.T. Czernuszka

Dr. R.I. Todd

Dr. M.L. Jenkins

Dr. P.J. Warren

Dr. S.D. Kenny

Dr. P.R. Wilshaw

Administrator

Mr. W.R.C. Briant

* emeritus

Senior Research Fellows

Dr. G.R. Booker	<i>OCAMAC Senior Fellow*</i>	Dr. J.W. Martin	<i>OCAMAC Senior Fellow*</i>
Dr. M.R. Castell	<i>Royal Society Research Fellow</i>	Dr. G. Möbus	<i>EPSRC Advanced Fellow</i>
Dr. J. Coyle	<i>OCAMAC Senior Fellow</i>	Dr. J.P. Northover	<i>Senior Research Fellow</i>
Dr. D.T. Goddard	<i>Wolfson Industrial Fellow</i>	Dr. O.V. Salata	<i>Senior Research Fellow</i>
Dr. P.S. Grant	<i>Royal Society Research Fellow</i>	Dr. P. Schumacher	<i>EPSRC Advanced Fellow</i>
Dr. G.W. Grime	<i>Senior Research Fellow</i>	Dr. C.B. Scruby	<i>Wolfson Industrial Fellow</i>
Dr. C.G. Harkins	<i>Linacre College Industrial Fellow</i>	Dr. G. Taylor	<i>Senior Research Fellow</i>
Dr. B.J. Inkson	<i>Royal Society Research Fellow</i>	Dr. D. Veseley	<i>OCAMAC Senior Fellow</i>
Dr. O.V. Kolosov	<i>EPSRC Advanced Fellow</i>	Dr. A.J. Wilkinson	<i>Royal Society Research Fellow</i>

Research Fellows

Dr. C. Allen	Dr. P. Hoffmann	Dr. C. Nörenberg
Dr. K.H. Baik	Dr. E. Holland	Dr. H. Nörenberg
Dr. J. Barghout	Dr. M. Huang	Dr. S. Noronha
Dr. V. Bliznyuk	Dr. B. Huey	Dr. I. Oleinik
Dr. V. Burlakov	Dr. S. Jordan	Dr. D. Ozkaya
Dr. P. Cizek	Dr. M.E. Keeble	Dr. I.G. Palmer
Dr. A. Cock	Dr. V. Kutepova	Dr. E. Palsgard
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Dr. D. de Kerckhove	Dr. R. Langford	Dr. S. Senkader
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Dr. B. Henry	Dr. J. Moore	Dr. T. Zhai
Dr. S. Hirosawa	Dr. A.P. Newbery	Dr. Y. Zhang
Dr. J. Hoekstra	Dr. Duc Nguyen Manh	

Part II Students

Metallurgy & Science of Materials

Azam, S.
 Barnes, J-P.
 Boon, P.
 Campbell, K.
 Cawkwell, M.
 Currie, D.
 Fletcher, H.
 Goodall, R.
 Hinchcliffe, C.
 Hogwood, A.
 Horbury, F.
 Ingram, J.
 Johnson, N.
 Mace, J.
 McGuigan, A.
 Speller, S.
 Taor, S.
 Willis, M.

Engineering and Materials Science

Chapman, R.T.G.
 Do, B.H.
 Edwards, E.G.
 Lorimer, E.G.
 Nawas, R.
 Oliver, R.A.
 Sonakul, A.
 Tsikouras, G.

Materials, Economics and Management

Abrahams, C.S.
 King, T.A.
 Miller, K.L.

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Mrs. K. Fewings	Mr. J. Richardson	Mrs. A. Wallin-Ashcroft
Mr. J. Forsdyke	Mrs. L. Richmond	Mr. L. Walton
Mrs. P. Gordon	Mr. W. Seager	

Research Students

Probationer Students

Allsop, N. (EPSRC / St. Annes Scholarship)	Maruyama, N. (Nippon Steel Corporation)
Brown, G. (CASE: Colebrand Ltd.)	Mason, D. (EPSRC / Applied Materials Linacre Scholar)
Burman, T. (CASE: National Power)	Ramanujan, C.S.
Dimitriou, K.	Rayment, T. (EPSRC / St. Cross Scholarship)
Jones, V. (EPSRC / St. Annes Scholarship)	Saunders, S. (CASE: National Physical Laboratory)
Kim, H.S.	Vaumousse, D. (CASE: Alcan International Ltd.)
Lozano-Perez, S. (EPSRC / St Annes Scholarship)	Wilkinson, S. (EPSRC / Guy Newton Wolfson Scholar)
Manson-Whitton, C.D.J. (Luxfer Ltd.)	

D.Phil.

Abraham, M. (EPSRC)	Kirov, K. (Toppan Printing Co.)
Abraham, M.H. (self-supporting)	Lee, H.K.(Self Supporting)
Balmer, B. (CASE: Merck Ltd.)	Lim, H.S. (National University of Singapore Scholarship)
Brand, A. (CASE: Cookson Industrial)	Llewellyn, H. (CASE: Sprayforming Developments Ltd)
Browne, D.J. (self supporting)	Maensiri, S. (Thai Government)
Campbell, P.J.D. (CASE: BNFL)	McKay, B. (CASE: London and Scandinavian)
Chandrapalan, P. (CASE: National Power)	Nakamura, H. (Sanyo Electric Co., Japan)
Chilton, A. (CASE: Alcan)	Naylor, M.J. (EPSRC)
Coates, M. (EPSRC)	Nicol, A. (EPSRC/Magnox Electric)
Cockfield, T. (CASE: Alcan)	Ortiz-Merino, J.L. (Mexican Government)
DeMoraes, A. (Nordiko Ltd)	Ormston, M.W. (CASE: Teer Coatings Ltd)
DeArdo, I. (Self-supporting)	Pak, S.J. (Self-supporting)
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Erlat, A.G. (Toppan)	Porfyraakis, K. (EPSRC/ICI Acrylics, Wilton)
Fenn, M.J. (EPSRC)	Ruitenbergh, G. (EPSRC)
Fuller, M.J. (CASE: Lucas Advanced Engineering Centre)	Sasaki, S. (Okinaga Scholarship, Wadham College)
Gladstone, T.A. (EPSRC)	Seerden, K. (EPSRC)
Gledhill, S. (EU)	Sha, G. (Alcan International Ltd)
Grimble, R. (EPSRC)	Shin, M. (CASE: Alcan)
Han, D-S. (Hyundai Motor Co., Korea)	Simmons, P. (CASE: T&N Technology)
Hedges, M.K. (EPSRC)	Spindura, J. (EPSRC)
Holloway, M. (EPSRC)	Steer, T. (EPSRC)
Howells, R.O. (EPSRC / Volvo Aero Corporation)	Trancik, J. (Rhodes Scholarship)
Hwu, K-L. (Self-supporting)	Valladares, A. (DGAPA, Mexico)
Ishii, H.	Wu, H. (Research Assistant)
Jeffery, S. (EPSRC)	Yoo, K-D. (British Council/Hyundai Electronics, Korea)
Jiansirisomboon, S. (Thai Government)	Zhang, L. (ORS & University)
Kang, K. (Self-supporting)	
Kara, H. (Turkish Government)	

Visiting Academics

Mr. N.J. Akram (Visiting student from University of Manchester)
Dr. P.H. Clifton (Seagate Technology Ltd., Ireland)
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Mr. F. Gomez-Cuevas (Visiting student from Escuela Superior de Ingenieros, Seville, Spain)
Professor R. Howson
Professor K. McKenzie (Industrial Research Ltd., New Zealand)
Dr. Suk-Hwan Kim (Yonsei University, Seoul, Korea)
Dr. Byung-Chul Ko (Inha University, Korea)
Professor M. Grant Norton (Washington State University, USA)
Professor L-M. Peng (Chinese Academy of Sciences, Beijing, China)
Professor B. Robertson (University of Nebraska, USA)
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Dr. F. Tillwick (University of Bremen, Germany)
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Dr. W. Zeng (Chinese Academy of Sciences, Shanghai Institute of Ceramics)
Dr. Xiya Zhou (South China University of Technology, Guangzhou, China)

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AlphaFry Ltd	National Power
BNFL	National Physical Laboratory
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Corus	NERC
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Magnox Electric	

Profiles of Academic Staff

Dr. Hazel Assender

Linacre College

Lecturer in Materials

DERA SMC Fellow

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 characterisation and modification. Modelling spans a wide range from atomistic modelling of crystal structure through mesoscale microstructural modelling and finite element continuum level simulations.

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, polycrystalline layers. Composition, geometry, interfaces, defects, phase separation, atomic ordering. Relationship between growth method, structures, optical and electrical properties. Lasers, detectors, polysilicon emitter bipolar transistors.

Mr. Richard Briant

St Cross College

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.

Professor Andrew Briggs

Wolfson College

Professor of Materials

Study of surfaces of materials over a logarithmic range of depth scales from a fraction of a millimetre to the top layer of atoms or molecules, using a range of acoustic and scanning probe microscopy techniques, including time-resolved and quantitative acoustic microscopy, surface Brillouin spectroscopy, ultrasonic force microscopy, variable temperature ultrahigh vacuum scanning tunnelling microscopy.

- Holliday Prize, Institute of Materials, 1984

Professor Clive Bradley

Wolfson College

Visiting Professor

Electronic materials and systems, semiconductors, research and development management and strategy.

[Advisor to Sharp Laboratories of Europe Ltd.]

Professor Richard Brook
St Cross College

Professor of Materials

Processing and properties of ceramic materials.

[Currently Chief Executive at the Engineering
and Physical Sciences Research Council.]

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. Use of neutron reflection and ion beam depth profiling techniques for studying surfaces and interfaces.

Professor Brian Cantor FREng
St Catherine's College

Cookson Professor of Materials
Head of Department

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
Wolfson College

Royal Society University Research Fellow

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

Dr. Alfred Cerezo
Wolfson College

Lecturer 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.

Professor Jack Christian FRS
St Edmund Hall

Emeritus Professor

Deformation of bcc metals and alloys, martensitic transformations, martensitic and epitaxial interphase interfaces, study of deformation twinning.

- Platinum Medal, Institute of Materials
- Acta Metallurgica Gold Medal
- Mehl Medal, AIME
- Gold Medal, Japan Institute of Metals

Professor David Cockayne FRS
Linacre College

Professor 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.

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, dry delivery systems and hierarchically controlled structures.

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

Professor Brian Eyre FEng.
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.

Dr. Patrick Grant
Linacre College

Royal Society University Research Fellow
Director of Oxford Centre for Advanced
Materials and Composites

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

Senior Research Fellow

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

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.

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
St Edmund Hall

Professor of Materials

Modelling and understanding fundamental solidification processes. This has included work on eutectics, peritectics, cellular and dendritic growth. The fundamental understanding has been applied to casting processes. Recent work includes an experimental and theoretical study of twin roll casting.

- 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.

Dr. Beverley Inkson

Royal Society University Research Fellow

Mechanical properties of nanostructured materials. Indentation, in-situ and high resolution electron microscopy techniques are used to evaluate deformation and failure mechanisms of nanocomposite intermetallics and ceramics, multilayers and thin film coatings.

Dr. Mike Jenkins
Jesus College

Research Lecturer

Radiation damage, transmission electron microscopy, metal matrix composites, ceramic nanocomposites, phase stability under irradiation. Recent work has focused on fundamental mechanisms of radiation damage, especially displacement cascade processes, and mechanisms of embrittlement of pressure vessel steels.

Dr. Steven Kenny

Lecturer in Materials

Application of materials modelling at the atomistic level to the description of real materials. Development of ab-initio methods for the description of materials.

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.

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.

Dr. Günter Möbus

EPSRC Advanced Fellow

Characterisation of materials on the atomic scale. Development of improved electron microscopy techniques for mapping of strain and retrieval of crystal defect structures using high-resolution electron microscopy in combination with nanobeam electron diffraction and analysis. Advanced studies on statistical image processing and dynamical simulations of electron diffraction.

Dr. Peter Northover
St Catherine's College

Senior Research Fellow

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.

Dr. Keyna O'Reilly
Pembroke College

Lecturer in Materials

Solidification processing of advanced materials and thermal analysis of phase transformations, covering a wide range of materials including Al alloys, intermetallics, biomaterials, and solder alloys. Currently developing new highly controllable techniques for simulating commercial solidification on a laboratory scale.

Dr. Amanda Petford-Long
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 kinetics (in-situ TEM annealing) in phase-change optical films and optical nanocomposite films.

Professor John Pethica
St Cross College

Professor of Materials Science

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.

- Sabbatical Chair, Sony corporation R&D, Japan, 1993-4
- Rosenhain Medal and Prize, Institute of Materials, 1997

Professor David Pettifor FRS
St Edmund Hall

Isaac Wolfson Professor of Metallurgy
Director of Materials Modelling Laboratory

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

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

Dr. Steve Roberts
St Cross College

Lecturer in Materials

Mechanical behaviour of brittle 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. Robert Rudd
Linacre College

Lecturer in Materials

Multi-scale simulation of materials. Modelling of mechanical, dynamical and transport properties of MEMS microsystems and other mesoscopic systems based on concurrent simulations at the angstrom, nanometre and micron scales. Characterization of micro-crack propagation in semiconductors. Nanotribology. Theory of unconventional superconductors.

Dr. Peter Schumacher
Fellow

EPSRC Advanced

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.

Professor George Smith FRS
Trinity College

Professor of Materials

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 Bilby Medal and Prize, 1985.

Professor Adrian Sutton
Linacre College

Professor of Materials

Modelling of materials at the atomic and microstructural levels : Computational materials synthesis. STM and surface structure of Mott-Hubbard insulators. Mechanical and electrical properties of nanocontacts. Interfaces. Dislocations. Microstructural evolution due to phase transformations and plasticity.

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 g-TiAl and various B2 compounds. Relating yield stress and strength to the properties of dislocations. Measuring elastic constants.

Professor John Titchmarsh
St Annes

**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. Surface engineering. 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. Paul Warren

Lecturer in Materials

Nanostructured materials. Non-equilibrium processing combined with structural and chemical characterisation on the nanometre scale using a range of microanalytical techniques. Materials under investigation range from conventional precipitation hardened aluminium alloys through to novel amorphous, nanocrystalline and nanoquasicrystalline alloys.

Professor Mike Whelan

Emeritus Professor

Linacre College

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

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

Dr. Angus Wilkinson

Royal Society University Research Fellow

Corpus Christi College

Mechanics at the microscopic scale, both experimental and modelling. Modelling of fracture and fatigue and validation of modelling approaches by comparison of predicted microscopic stress distributions with those revealed experimentally by SEM based diffraction techniques.

Dr. Peter Wilshaw

Lecturer in Materials

St Anne's College

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.

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The image shows fatigue damage (cracks and persistent slip bands) in an Al-Li alloy (8090). The material has a fine elongated grain structure as a result of its processing route: spray casting then extrusion. Fatigue damage is seen to initiate at many sites within some grains but is absent from others. Electron back scatter diffraction shows that grains of specific orientations are preferential sites for initiation of fatigue cracks.

Dr. Tongguang Zhai, Dr. Angus Wilkinson and Dr. John Martin.

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 DERA Pyestock)

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.

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.

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.

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)

Frictional welding of intermetallics

*Dr. B. Inkson, Dr. P. Threadgill**

The joining of oxide dispersion strengthened intermetallic alloys by friction welding is being investigated, paying particular attention to the behaviour of the nanometre sized ceramic particles and the evolution of texture during the friction welding process. (*The Welding Institute, Cambridge)

Transition metals in TiAl

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

Microstructures of γ + β + 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)

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 multi-component thin films

Dr. B.J. Inkson, Dr. G. Möbus, Professor E. Arzt, 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 electron microscopy and FIB down to the atomic level. (*Max-Planck-Institut für Metallforschung, Stuttgart, Germany) (Funded by The British Council, DAAD and The Royal Society)

Amorphous and nanocrystalline alloys

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

Amorphous and nanocrystalline alloys are being fabricated by rapid solidification processing. The resulting microstructures are being characterised by TEM and APFIM. The effect of different alloying elements upon the phase stability of the resulting nanocomposite microstructures is being investigated. (Funded by EPSRC and in collaboration with Carpenter Technology and DERA Farnborough)

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

*T. Steer, Dr. B.J. Inkson, Dr. R. Langford, Dr. Th. Wagner**

Surface plastic deformation in multilayers and nanocomposites, generated by nanoindentation, scratch tests and abrasion, are being systematically sectioned and characterised in 3D by FIB. (*Max-Planck-Institut für Metallforschung, Stuttgart, Germany) (Funded by EPSRC and The Royal Society)

Nanoscale deformation of materials quantified by TEM nanoindentation

A.N. Other, 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. (Funded by EPSRC and The Royal Society)

Quasicrystalline nanocomposites

Dr. S.H. Kim, Dr. B.J. Inkson, Dr. P.J. Warren, Professor D.H. Kim, Professor W.T. Kim**

Novel high strength quasicrystalline nanocomposites are being developed using a range of processing techniques including mechanical alloying, casting and meltspinning. Their microstructures are being characterised by high spatial resolution electron microscopy and atom-probe field ion microscopy. (*Yonsei University, Seoul)

III - MECHANICAL PROPERTIES OF STRONG SOLIDS, METALS AND ALLOYS

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

Professor J.W. Christian, 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.

Physical properties of Li-Mg alloys

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

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

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 DERA)

Fundamentals of 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 initiation and early growth of fatigue cracks. (Funded by EPSRC and The Royal Society)

Growth of short fatigue cracks in Al-Li alloys

Dr. T. Zhai, Dr. A.J. Wilkinson, Dr. J.W. Martin, Professor B. Cantor

The crack growth rate reduction caused by interaction of dislocations ahead of short fatigue cracks with grain boundaries, is being studied. The effects of precipitate distributions and local crystallographic texture on crack growth rates will be determined for 8090 and UL30 alloys. The aim is to identify microstructures which impede the early growth of fatigue cracks. (Funded by EPSRC in collaboration with British Aluminium Plate, DERA Farnborough and Westland Helicopters)

Carbide cracking and the brittle-ductile transition in ferritic steels

M. Coates, Dr. S. Noronha, Dr. S.G. Roberts

The effects 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)

Variable temperature nanoindentation

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

A nanoindenter with controllable test temperature has been implemented. It is used to study time dependent deformation in sub-micron samples.

Mechanical properties of semi-solid slurries

D.S. Han, 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. (Funded by Hyundai Motors in collaboration with KIST)

Mechanical properties of squeeze cast Al alloy composites

M. Fuller, Dr. P. Schumacher, Professor B. Cantor

Squeeze casting is being used to manufacture Al alloy near net-shape components containing local reinforcements of various types. A combination of mechanical testing and numerical modelling is being used to determine the composite mechanical properties and to optimise the resulting material. (Funded by EPSRC and Lucas)

Diffusion bonding of zirconium alloys

P.S. Hill, Dr. R.I. Todd, Dr. N. Ridley**

Diffusion bonding is a solid state joining method for metallic alloys. Advantages include minimal distortion of the product and the ability to join thick sections. Diffusion bonding is already used extensively for titanium alloys and duplex stainless steels. The aim of this project is to extend this useage to zirconium alloys, which are employed in nuclear power generation and chemical plant. Preliminary experiments have demonstrated the feasibility of diffusion bonding zirconium, and the research is now concentrating on establishing the mechanisms of bond formation, so that modelling can be used to predict bonding conditions and surface treatments suitable for commercial application. (*University of Manchester) (Funded by EPSRC and Rolls Royce & Associates Ltd.)

Microstructure-property relationships in commercial superplastic 7475-aluminium alloys

*Dr. A.N. Other, 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)

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.)

Mechanical properties of the bond coat in thermal barrier coatings

R.O. Howells, Dr. R.I. Todd, J. Wigren, P. Bengtsson**

The mechanical properties of air plasma sprayed NiCoCrAlY bond coats are being investigated, and the results are being used to model the thermal residual stresses which accrue during deposition and subsequent thermal cycling. Direct measurements of the thermal residual stresses are being made for comparison by measuring the curvature of coated substrates during thermal cycling. (*Volvo Aero Corporation)

Measurement and development of residual stresses in coatings

*S. Saunders, Dr. R.I. Todd, Dr. P.M. Mummery**

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)

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The figure shows a scanning electron microscope image of a cross-section through a pore in a UO_2 single crystal. Pores are remnants of the spectacular grain growth process and can vary in size from a few hundred nanometres to tens of microns. During the high temperature sintering process the trapped pores adopt the equilibrium crystal shape for the UO_2 fluorite structure which is bound by $\{111\}$ and $\{001\}$ faces, and these can be seen in the micrograph. Facetting between the faces in the larger pores is also a distinct feature in these images. By comparing the relative surface areas the surface energy ratio can be determined. It is found that the $\{001\}$ to $\{111\}$ surface energy ratio is 1.2.

Dr. Martin Castell

B. Non-Metallic Materials

I - CERAMICS AND COMPOSITES

Properties of nanophase ceramic coatings

S. Jiansirisonboom, Dr. P.S. Grant, Dr. S.G. Roberts

Alumina/ SiC nanocomposite coatings are being made by plasma spraying, and their microstructures and mechanical properties investigated. (Funded by Thai Government)

The influence of heat treatment on the strength of ceramic nanocomposites

H. Wu, Dr. S.G. Roberts

Annealing increases the strength of alumina/silicon carbide ceramic nanocomposites. To investigate this, we are using acoustic and Hertzian indentation techniques to investigate the effects of heat treatment on the defect population and strength in these materials before and after surface machining. (Funded by EPSRC)

Nanocomposite ceramics for technical applications

H. Kara, H. Wu, Dr. S.G. Roberts

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. This is part of a BRITE-EURAM programme in collaboration with Morgan Matroc, Limerick University, Belgian Ceramic Research Centre, University of Valenciennes and Treibacher Schleifmittel. (Funded by BRITE-EURAM and Turkish Government)

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 single-crystalline, 3-D networks, giving unusual properties. (*In collaboration with the Ioffe Physical-Technical Institute, St Petersburg, Russia, supported by the Royal Society)

Chemical synthesis of alumina-SiC nanocomposites

Dr. W. Zeng, Dr. R.I. Todd

Alumina/SiC nanocomposites are being fabricated using a chemical route in which alumina is derived from an inorganic aluminium salt to produce the matrix. The influence of the processing details on microstructural characteristics such as grain size and SiC particle position are being studied, with the aim of understanding the role of the gamma to alpha phase transition in determining the final microstructure. (Funded by The Royal Society)

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 in glasses and ceramics

Y. Bisrat, Dr. S.G. Roberts

A new technique based on Hertzian indentation is being used to quantify the effects of treatments which produce strengthening in glass and ceramics by introducing a surface compressive layer. (Funded by Merton College and in collaboration with Pilkington Glass and Morgan Matroc)

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.

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)

Thermal shock of alumina-SiC nanocomposites

S. Maensiri, Dr. S.G. Roberts

We are examining the thermal shock resistance and failure mechanisms in sintered alumina - silicon carbide "nanocomposite" ceramics. (Funded by the Thai Government)

II - BIOMEDICAL MATERIALS

Studies on the precipitation of calcium phosphate

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

The kinetics of calcium phosphate precipitation are being determined and the products analysed. X-ray diffraction techniques and modelling are being used to determine the phases present, their proportions, morphologies and preferred orientations. Comparison with other techniques will be made throughout. (*Philips Research Labs)

In situ formation and electrodeposition of active coatings

S. Wilkinson, 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)

Macro-assembled spheres of apatite

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 and Thai Government)

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.)

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)

Mechanical properties of biocomposites

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.

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)

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.

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)

Ab initio calculations of biochemicals and their interactions

Dr. J.T. Czernuszka, Professor D.G. Pettifor, Dr. S. Sasaki, Dr. H.E. Assender

Density functional theory and force fields are being used to calculate the structure and vibration spectra of biomolecules. Interaction(s) of these biomolecules with calcium ions and solid surfaces will be determined to predict how biomaterials will interact with the host tissue. (Funded by Okinawa Scholarship)

III - POLYMERS

The hierarchical structure of spider silk

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

Spider silk microstructures on the scale of 1 nanometer to 1 micrometer are being characterised by transmission electron microscopy / diffraction. Molecular modelling is being used to identify particular amino acid sequences that can account for the observed microstructural features, which in turn are associated with specific mechanical properties. (*Heriott-Watt University) (Funded by EPSRC)

The response of poly(vinyl alcohol) to humidity

J. Spindura, Dr. H.E. Assender

The control of water solubility in poly(vinyl alcohol) is achieved industrially using heat and chemical treatments, the effect of which are not fully understood. The uptake of water into the polymer prepared as films and fibres, and its effect on crystallinity and morphology as well as the effect of heat/crosslinking treatments upon this process is being examined. (Funded by EPSRC)

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 Chemical Engineering, Imperial College) (Funded by EPSRC)

Mesoscale modelling of processing rubber toughened polymers

K. Porfyrakis, Dr. H.E. Assender

A mesoscale model for predicting the microstructure of a rubber toughened polymer after typical processing treatments such as extrusion and injection moulding. The distribution and deformation of rubber toughening additives will be modelled using calculations of flow history during processing made from finite element models. (Funded by the EPSRC and ICI Acrylics)

Polymer adhesives with good interfacial bonding

Dr. H.E. Assender

A novel system is under development to enhance interfacial bonding in a polymeric adhesive system. The research includes characterisation of nanoscale interfacial defects, investigation of diffusion and demixing in polymer blends, encapsulation technology and mechanical testing of joints. (In collaboration with DERA)

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 aims to study the effect of molecular architecture on the diffusion process for a set of chemically identical polymers, and interpret this under the framework of the reptation model. (*Materials Science Centre, UMIST; **Department of Chemistry, Imperial College; ***Department of Chemical Engineering, Imperial College)

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)

Properties of macrozwitterions

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

Macrozwitterions have slightly different thin film and bulk structural properties compared to the parent homopolymer due to segregation of the oppositely charges end groups. The molecular structure and orientation can be drastically altered by application of external fields. This project aims to study the effects of applying an external field in controlling the structure within these thin film and bulk materials. (*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 is 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 National Power)

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)

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

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

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.

Development of ion-permeable membranes

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 National Power)

Polymer matrices for PMCs

K. Campbell, Dr. H.E. Assender

The development of toughened matrix resin systems for use in a wide range of polymer matrix composite materials. The addition of toughening materials into novel matrix systems is investigated, relating morphology with mechanical properties. (In collaboration with DERA)

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)

IV - PACKAGING MATERIALS

Deformation and fracture of polymer-glass nanocomposites

Dr. O. Kolosov, A. McGuigan, Dr. Y. Tsukahara, Professor G.A.D. Briggs, Dr. H.E. Assender*

Fracture properties of polymer-glass nano-composites on submicrometre level are studied using surface Brillouin spectroscopy and ultrasonic force microscopy. (*Funded by and in collaboration with The Toppan Printing Company)

Characterisation of glassy barrier films on PET substrates

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

The microstructure of PET/glass films is being studied in order to correlate the gas transmission properties with defects produced during fabrication and handling. High resolution TEM and SEM, Atomic Force Microscopy and microanalysis techniques are being used to study the glass layer, and observations of defects such as local cracking, porosity and impurity contamination are proving valuable in explaining the barrier layer properties of these composite packaging materials. (Funded by and in collaboration with 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)

Polymer surfaces

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

The topography, adhesion and mechanical properties of polymer surfaces will be examined by combination of number of techniques to a series of model systems. Techniques will include SPM, SBS and XPS. The surface will be considered as a precursor to an interface, and various surface treatments and deposition routes will be examined. (Funded by The Toppan Printing Company)

Prediction and measurement of crystallinity at a polymer surface

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

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

Reactive, dual target sputtering is being used to deposit Al(X) oxide 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. (Funded by and in collaboration with The Toppan Printing Company)

Polymer interfaces

Dr. C.S. Deng, Dr. H.E. Assender

The interfaces in nanocomposite materials used for packaging are under examination. In particular, the role of the adhesive or boundary layers that may be used to enhance the deposition of subsequent layers is investigated, as well as the role of such interfaces and interfacial layers in the performance of the composite as a barrier material. (Funded by The Toppan Printing Company)

Plasma deposition of polymer layers

*J. Mace, Professor G.A.D. Briggs, Dr. H.E. Assender, Dr. Y. Tsukahara**

Thin polymer films are deposited and polymerised on a PET substrate. Dielectric films find application in food packaging, which must be impermeable to oxygen and water and also transparent to light and microwaves. The degree of polymerization and surface roughness can be characterized by various methods including AFM, ATR FTIR and MALDI. By careful choice of different monomer precursors and by changing the plasma conditions it may be possible to refine the deposition process to produce a thin film with optimum properties. (*Funded by and in collaboration with The Toppan Printing Company)

Post deposition improvement of nanocomposite oxide layer

*N.B. Johnson, Professor G.A.D. Briggs, Dr. C.R.M. Grovenor, Dr. Y. Tsukahara**

The aim is to improve the permeation properties of an SiO_x , AlO_x or ITO (Indium Tin Oxide) layer on a PET substrate after deposition. The oxide layer is typically only tens of nanometres thick and has a rather loose amorphous structure. It is believed that a treatment that tightens this structure would inhibit the permeation of oxygen and water vapour. Various processes are being evaluated. The effects of the treatments on the mechanical and permeation properties of the film will be characterised using a variety of techniques. (*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. D. Vesely, 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)

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SEM micrograph showing a section through a high density field emitter array. These devices, produced by a novel non-lithographic technique are ultimately intended for use as cold cathodes in flat screen displays.

Dr. Ed Holland

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.

Development of practical conductors and devices from high temperature superconducting ceramics

Dr. J.C. Moore, Dr. X. Zhou, 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 practical conductors which are capable of carrying significant currents at liquid nitrogen temperatures and much larger currents at lower temperatures. Current work is concentrating on the development of spray pyrolysis and 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. (*Department of Engineering Science) (Funded by EPSRC)

Microstructural and microelectronic characterisation of superconducting materials

Dr. J. Moore, B. Balmer, T. Gladstone, R. Goodall, C.J. Salter, Dr. C.R.M. Grovenor

Superconducting ceramic samples fabricated in bulk and thin film form are being characterised by 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 in a number of collaborators, and correlation of these features with critical current measurements. High resolution and analytical TEM, XRD texture analysis, electron microprobe and orientation imaging microscopy techniques are being used extensively. (Funded by EPSRC)

Fabrication of thin films of superconducting ceramics

Dr. A. Jenkins, Dr. C. Stevens*, Dr. V. Boffa**, Dr. C.R.M. Grovenor, Professor D. Edwards*, Professor D. Dew-Hughes**

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. Dr Boffa's group are depositing YBCO film on Oxford substrates. (*Department of Engineering Science; **ENEA Frascati) (Funded by EPSRC and in collaboration with ENEA Frascati, Department of Physics, Kings College London, Department of Engineering Science, Oxford, Department of Metallurgy, University of Cambridge)

Microwave device fabrication from superconducting thin films

Dr. A.P. Jenkins, Dr. C. Stevens*, Professor D. Dew-Hughes*, 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 a variety of 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. (*Department of Engineering Science) (Funded by EPSRC and in collaboration with WSIL Ltd, BBC, Hymatic Ltd., Birmingham University Portsmouth University, Kings College London and Department of Engineering Science)

Properties of metallic substrates for superconducting tapes

T. Gladstone, R. Goodall, Dr. X. Zhou, Dr. J. Moore, Dr. C.R.M. Grovenor

The thermal/mechanical properties of nickel, silver and silver alloy substrates are being investigated to identify the most promising material for use in Tl-1223 superconducting tapes. High quality cube textured Ni and <110> textured Ag substrates are being produced, and oxide buffer layers growth by spray pyrolysis, solution growth, electrodeposition and sputtering. The texture relationship between the metal substrate and the superconducting phase is a central aspect of this work. (Funded by EPSRC and in collaboration with ENEA Frascati)

Analysis strategies for assessing textured superconducting artefacts

S. Speller, Dr. E. Maier, Dr. C.R.M. Grovenor*

A range of techniques are being developed to assist in the assessment of coated superconducting samples, including; inductive probe mapping, Jc/strain measurements and measurements of percolation paths in EBSD data. (*Oxford Instruments) (Funded by EPSRC)

II - SEMICONDUCTOR MATERIALS

Semiconductor quantum dots

Dr. P. Möck, Dr. G.R. Booker, Dr. P.R. Wilshaw, Dr. P. Klipstein, Professor R.J. Nicholas**

InSb quantum dots embedded in either InAs or GaSb are grown by MOVPE and assessed by TEM, atomic force microscopy, photoluminescence, Raman spectroscopy and electrical measurements. Conditions are optimised to give high luminescent emission in the near infra-red and mechanism are determined. (*Clarendon Laboratory, Oxford) (Funded by EPSRC)

Impurity-dislocation interactions in silicon

Dr. P.R. Wilshaw

The electrical properties of individual dislocations are being investigated using the SEM-EBIC and DLTS methods. The mechanism by which very low concentrations of impurities, including hydrogen, can markedly change the electrical recombination efficiency of these defects is being studied and the measurements used to investigate the gettering efficiency of dislocations at very low impurity concentrations.

Locking of dislocations by oxygen in Si wafers

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

The oxygen present in Czochralski Si wafers contributes significantly to the strength of the material by locking any dislocations present. The size of this effect is being investigated as a function of oxygen concentration and anneal times and temperature. (*MEMC, Novara, Italy)

Secondary electron mapping of doped regions in semiconductors

Dr. M.R. Castell, Dr. A.J. Wilkinson, Dr. P.R. Wilshaw

The secondary electron (SE) signal in an SEM is used to produce 2-dimensional maps of doped regions in silicon and III-V semiconductors. SE images of cross-sections of doped heterostructures and laser devices reveal the type and extent of doping. Quantitative information about the observed contrast has been obtained experimentally. A model has been proposed and is being developed to account for the effect.

Investigation of strained epilayers using electron diffraction in the SEM

Dr. A.J. Wilkinson

The factors controlling the strain relaxation of misfitting epitaxial layers grown on planar and patterned substrates are being examined. Electron channelling contrast imaging is used to image and characterise the groups of dislocations generated during relaxation. Techniques for probing local elastic strain fields using electron back scatter diffraction patterns are being developed. (Funded by The Royal Society)

Dielectric breakdown of thin SiO₂ films

*S. Jeffery, Professor J.B. Pethica, C.J. Sofield**

The dielectric breakdown strength of 1-5nm thick SiO₂ films is measured locally with a conducting probe in a Nanoindenter. It is shown that the breakdown field is pressure sensitive. Models of breakdown are under development. (*AEA Harwell)

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 bipolar transistors by using selective chemical etching in combination with AFM and TEM techniques. The method is being developed for application to shallow p-n junctions.

Quantum wires and dots

Dr. J.L. Hutchison, S. Gledhill, N. Allsop, Professor P.J. Dobson, Dr. O. 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)

Diffusion of fluorine in silicon

Dr. G.R. Booker, Dr. C.D. Marsh, Dr. G. Nash, Professor P. Ashburn**

Single crystal, polycrystalline and amorphous silicon specimens are being implanted with fluorine and annealed. TEM structural results and SIMS fluorine concentration profiles are being used to deduce fluorine diffusion data and mechanisms. (*Electronics Department, Southampton University) (Funded by EPSRC)

Nucleation of dislocation sources in $\text{Ge}_x\text{Si}_{1-x}$ layers on Si

Professor Sir Peter Hirsch, Dr. S. Jiao, Professor D.D. Perovic***

The nature of dislocation sources (called "double half loops") generated at the interface between $\text{Ge}_x\text{Si}_{1-x}$ layers and the Si substrate is being studied by weak beam TEM, and a mechanism for their formation is being developed. (*Argonne National Laboratory, Argonne IL, USA; **Department of Metallurgy and Materials Science, University of Toronto, Canada).

In-situ doped polysilicon layers

Dr. C.D. Marsh, Dr. G.R. Booker, A.I. Abdul-Rahim, Professor P. Ashburn**

TEM structural studies of in-situ doped polysilicon layers deposited on silicon wafers using a UHV cluster tool system are being performed and the results correlated with the deposition conditions and electrical measurements. (*Electronics Department, Southampton University) (Funded by EPSRC)

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 wafer 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. The work has application to high performance polysilicon emitter bipolar transformers. (*Electronics Department, Southampton University; **Mitel Inc., Swindon; ***Electrical Engineering Department, Waterloo University, Canada) (Funded by EPSRC)

Scanning Infrared Microscopy - development and applications

Dr. G.R. Booker, Dr. P.R. Wilshaw, Dr. Z.J. Laczik, Dr. P. Torok**

A high performance polarising scanning infrared microscope operating in transmission and reflection is being developed. It is being used to investigate defects in semiconductor specimens, e.g. dislocations and precipitate particles (*Department of Engineering Science)

Epitaxial electrodeposition of semiconductor quantum dots

Dr. J.L. Hutchison, Professor I. Rubinstein, Dr. G. Hodes**

Electrodeposition of CdSe and CdS from non-aqueous solutions containing Cd^{2+} and elemental Se or S onto Au or Pd substrates results in nanocrystals with wurtzite structure, about 5 nm in diameter. The size and structure of the crystallites may to some extent be controlled by lattice mismatch with the substrate. The materials are being characterised by electron optical and other techniques. (*In collaboration with the Weizmann Institute, Israel)

The mechanical strength of CZ silicon wafers

D. Currie, Dr. S. Senkader, K. Jurkschat, Dr. R. Falster, Dr. P.R. Wilshaw*

The influence of oxygen precipitates on the mechanical yield of silicon wafers is being investigated. The effect of precipitate size, density and different heat treatments is being investigated. It is hoped that stronger wafers will be produced and this will be beneficial to the silicon semiconductor industry. (*MEMC, Novara, Italy)

III - MAGNETIC MATERIALS

Growth and characterisation of magnetic multilayer systems for magnetic and magneto-optic recording

Dr. A.K. Petford-Long, Dr. J.L. Hutchison, K. Kang

The structure and composition profile of thin multilayer films with applications as magneto-optic recording are being studied on the atomic scale using HREM, STEM microanalysis and atom-probe microanalysis, for correlation with the magnetic properties. The magnetic domain structure is being characterised using Lorentz microscopy in the 4000EX TEM. The films are being grown by UHV evaporation or magnetron sputter deposition. (Funded by The Royal Society)

Microstructure and resistivity of multilayer films

Dr. A.K. Petford-Long, Dr. J.F. Gregg, M. Fenn*

The validity of a model for the resistivity of non-magnetic and magnetic multilayer films is being tested experimentally. The theory has so far been applied to Cu/Nb multilayers and this is being extended to other systems. (*Clarendon Laboratory) (Funded by EPSRC)

Microstructure and magnetic structure of spin-valves

Dr. A.K. Petford-Long, Dr. H. Laidler, Professor K. O'Grady**, Dr. X. Portier****

The microstructure and magnetisation reversal mechanisms of spin-valve and spin-tunnel junction devices 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 Exeter; **Univ. of Wales, Bangor; ***University of Caen) (Funded by Seagate Technology and EPSRC)

Studies of patterned magnetic thin films

Dr. A.K. Petford-Long, Dr. A. Toporov, Dr. S.M. Thompson, R. Pickford**

Thin magnetic films grown by sputter deposition and by molecular beam epitaxy are being patterned to form arrays of magnetic dots. Their magnetic domain structure and magnetisation processes are being studied by Lorentz microscopy. (*Department of Physics, University of York) (Funded by EPSRC, The Royal Society and NATO)

Surface engineering of layered films for magnetic sensor applications

*M.W. Ormston, Dr. A.K. Petford-Long, Dr. D.G. Teer**

Magnetic layered films are being grown by magnetron sputter deposition and their interfaces are being modified in a controlled way by ion-bombardment to assess the usefulness of this technique for improving the magnetic and transport properties of the films. (*Teer Coatings Ltd) (Funded by EPSRC and Teer Coatings Ltd.)

Spin-tunnel junctions based on magnetic layered films

Dr. A.K. Petford-Long, Dr. D. Ozkaya, Dr. P. Shang, A. Hogwood, Dr. T.C. Anthony, Dr. J.A. Brug**

Spin-tunnel magnetic layered systems exhibiting giant magnetoresistance are being studied. 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)

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.)

Electromagnetic properties of high performance solenoid materials

*Dr. A.K. Petford-Long, S. Taor, H. Smith**

Fast acting solenoids are used in several diesel engine fuel injection systems, and it is important to control the magnetic properties. The project will involve microstructural analysis in Oxford of materials submitted to several heat treatments, and heat treatment and magnetic measurements will be carried out at Lucas in Solihull. (*Lucas Varsity)

IV - DISPLAY MATERIALS

Development of electroluminescent display based on organolanthanides

*S. Capecchi**, *Dr. A. Mosley***, *Dr. V. Christou****,
Dr. O.V. Salata

Organolanthanides are promising electroluminescent materials that can be used in flat panel displays. Their fundamental advantages such as pure green and red emission colours as well as possible 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 and then transferred to the CRL Ltd to be used in the manufacturing of display panels. (*Opsys Limited; **CRL Ltd.; ***ICL, Department of Chemistry) (Funded by Opsys Ltd.)

Material issues in degradation of OLEDs

*Dr. D.-G. Moon**, *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. (*Department of Engineering Science; **ICL, Department of Chemistry) (Funded by Opsys Ltd.)

Lanthanide Dendrimers as multifunctional materials for OLEDs

*Dr. J. Pillow**, *Dr. M. Halim**, *Dr. P. Burn***, *Dr. I.D.W. Samuel****, *Dr. V. Christou*****, *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, Durham University; ****ICL, Department of Chemistry) (Funded by Opsys Ltd.)

Transport properties and electronic structure of organolanthanides

*Dr. G. Maliaris**, *Dr. I.D.W. Samuel***, *Dr. V. Christou****, *Dr. O.V. Salata*

Knowledge of type and mobility of charge carriers in organic materials is important for design of effective OLED. It is also important to know the values of energy barriers to the charge injection from electrodes as well as HOMO-LUMO energy offsets at the organic-organic interfaces. Modelling of I-V-B characteristics, time of flight measurements, XPS and electrochemical methods are applied in order to get complimentary values of mobilities and energy levels. (*Department of Materials Science and Engineering, Cornell University; **Department of Physics, Durham University; ***ICL, Department of Chemistry) (Funded by Opsys Ltd. and Cornell University)

Development of a field emitter backlight for LCD's

Dr. Y-G. Li, *Dr. I. Gibb**, *Dr. P. Tyler***, *Dr. P.R. Wilshaw*

Large arrays of sub-micron field emitters are being fabricated in the pores of anodized aluminium deposited on a glass substrate. These substrates are then mounted in front of a phosphor bearing faceplate, sealed and evacuated by collaborators at CRL Ltd. Suitable driving electronics are being developed by Smiths Industries. The aim is to produce a working backlight for LCD illumination. (*CRL Ltd.; **Smiths Industries) (Funded by Foresight Challenge)

Investigation of current transport processes in nominally insulating materials

S. Azan, *Dr. P.R. Wilshaw*

This work involves injecting electrons into the conduction band of nominally insulating materials and measuring their properties. This work is relevant to field emission display devices.

Non-lithographic definition of sub-micron field emitter structures

Dr. E. Holland, Dr. Y-G. Li, Dr. P.R. Wilshaw

At present all 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)

Silicon field emitting tips

Professor G.D.W. Smith, Dr. P.R. Wilshaw

Silicon wafers are being etched to generate arrays of very sharp points such that field emission occurs at applied potentials of a few hundred volts. Such cold cathodes are an essential feature of the developing technology of vacuum microelectronics. We have recently shown that a thin porous silicon surface layer is able to improve the performance of these emitters by an order of magnitude. Working field emitter devices using porous Si are now being tested in different vacuum environments to assess their long term stability. (In collaboration with GEC, Hirst Research Centre) (Funded by EPSRC)

OLED interface engineering using ultra-thin inorganic layers

Dr. O. Renault, Dr. O. Kolosov, 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. (*Department of Engineering Science) (Funded by Opsys Ltd.)

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Electric arc spraying of steel onto shaped ceramic substrates is being investigated as a method of manufacturing tools and dies for application in a wide variety of industries. The key to successful manufacture of these complex steel shapes by spray forming is the on-line control of the residual stresses which are generated during manufacture to prevent warping, as well as ensuring that the steel spray accurately replicates any complex and fine scale topography. (Funded by EPSRC, The Ford Motor Co, Sulzer Metco and the Royal Society)

Dr. Patrick Grant

D. Processing

Spray formed Ni alloys

M. Hedges, T. Rayment, Dr. I.C. Stone, Dr. H.K. Seok, Professor B. Cantor, 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, Special Melted Products and Osprey Metals Ltd.)

Arc sprayed self lubricating coatings

H. Llewellyn, Dr. A.P. Newbery, Dr. P.S. Grant

Various grades of steel coatings containing a dispersion of graphite particulate are being manufactured by arc spraying. Coating microstructure is being characterised by microscopy and coatings are being wear tested in a special rig to assess their application in the off-shore oil industry. (Funded by EPSRC and Sprayforming Developments Ltd.)

Spray formed automotive tooling

*Dr. A.P. Newbery, Dr. Z. Djuric, Dr. P.S. Grant, Dr. S. Duncan**

Electric arc spraying of liquid steel droplets onto shaped substrates is being investigated for the rapid manufacture of dies for plastic injection moulding or stamping/pressing tools for a wide range of applications. Lead times are up to 10 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, Sprayforming Developments Ltd, Sulzer Metco and Ford Motor Co.)

Laser imaging and diagnostics in spray processes

*Dr. A.P. Newbery, Dr. P.S. Grant, Professor C. Webb**

A 40KHz Cu vapour laser is being used in conjunction with ultra fast video and photography to investigate the velocity and trajectory histories of molten metal droplets in a variety of spray processes. As well as novel developments in imaging techniques, the process measurements are related to operating variables and resulting sprayed microstructure. (*Department of Physics) (Funded by EPSRC)

Rapid steady state solidification of 1xxx, 3xxx and 6xxx series Al alloys

Dr. C.M. Allen, Dr. K.A.Q. O'Reilly, Professor B. Cantor

Phase selection in model and commercial 1xxx, 3xxx and 6xxx series Al alloys is being investigated using electron beam surface melting in order to simulate the high steady state growth velocities experienced in modern continuous casting techniques. (Funded by EPSRC and Alcan International)

Rapid steady state solidification of 6xxx series Al alloys

G. Sha, Dr. K.A.Q. O'Reilly, Professor B. Cantor

Phase selection in model and commercial 6xxx series Al alloys is being investigated using electron beam surface melting in order to simulate the high steady state growth velocities experienced in modern continuous casting techniques. (Funded by Alcan International)

Metallurgical soldering and bonding

A.D. Brand, Dr. K.A.Q. O'Reilly

Thermal and mechanical properties of metallurgical soldering and bonding materials are being investigated as a function of microstructure. The effect of initial microstructure, the thermal stability of the microstructure and its effect on the mechanical properties are being studied in a range of lead containing and lead-free materials. (Funded by EPSRC and Alpha Fry)

Low pressure squeeze cast alloys and composites

P. Simmons, Dr. P. Schumacher, Professor B. Cantor

A series of potential alloys for piston applications are being squeeze cast at low pressures to investigate structure and properties, and to develop lower cost squeeze casting methods. (Funded by EPSRC and Federal - Mogul)

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)

Twin roll casting of superplastic SPZ Zn-Al

*Dr. M. Yun, Dr. M.E. Keeble, 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.)

Twin roll casting of stainless steel and other ferrous alloys

*Dr. M. Yun, Dr. M.E. Keeble, Professor J.D. Hunt, P.G. Grocock**

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. (*Kvaener Metals) (Funded by EPSRC and Kvaener Metals)

Coupled eutectic growth in twin roll cast aluminium alloys

*T. Cockfield, Dr. M.E. Keeble, 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)

Spray formed Al alloys

Dr. I.C. Stone, Dr. I.G. Palmer, Dr. P.S. Grant, Professor B. Cantor

A 80kg Al spray forming plant is currently being installed 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. British Aerospace Military, GKN Westland Helicopters Ltd and DERA)

The downstream processing of twin roll cast aluminium alloys

*Dr. M. Yun, Dr. M.E. Keeble, 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)

Continuous casting of copper base alloys

*Dr. M. Yun, Dr. M.E. Keeble, 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)

Microstructural studies of Pb-Sn solder/PCB interactions

C. Langham, Dr. C.R.M. Grovenor, Dr. S. Gupta**

The stability of copper PCB tracks coated with commercial Ni, HASL, OSP and Pd protective coatings in contact with molten Sn-Pb solder is being studied in order to compare the performance of these barrier layers in wave soldering operations. (*Motorola ECID)

Second generation Ti MMCs

Dr. K.H. Baik, Dr. P.S. Grant, Dr. M.L. Jenkins, 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 (Funded by EPSRC, Rolls-Royce plc and DERA).

Manufacture of Ti MMCs

Dr. T.W. Kim, Dr. F.P. Dunne, Dr. Z.X. Guo**, Professor B. Cantor*

The manufacture of Ti MMCs is being controlled by modelling and experimental validation to understand the development of porosity, interface reaction, fibre fracture and other defects during hot consolidation. (*Department of Engineering Science; **Queen Mary Westfield) (Funded by EPSRC, Rolls-Royce and DERA)

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)

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 DERA Farnborough)

Grain refinement tolerance to Fe

*Dr. E.D. Manson-Whitton, Dr. K.A.Q. O'Reilly, M.R. Jarrett**

Control of intermetallic phase selection, together with modified quenching procedures after extrusion, is being investigated to allow increased productivity of extrusions while maintaining, or improving, surface quality of the product and increasing tolerance to Fe impurity. (*Luxfer Group)(Funded by Teaching Company Scheme)

Multicomponent alloys

Dr. B.C. Ko, F. Gomez Cuevas, 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. (Funded by British Council)

Surface quality of 6xxx series Al extrusions

*M. Willis, Dr. E.D. Manson-Whitton, Dr. K.A.Q. O'Reilly, M.R. Jarrett**

The effect of impurity content and homogenisation heat treatment on billet microstructure together with the resultant effect on surface quality of extrusions is being studied in 6xxx series Al alloys. (*Luxfer Group) (Funded by Luxfer Group Limited)

Novel manufacturing routes for Al products

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

Novel manufacturing technologies are being investigated for the manufacture of Al alloy products. (*Luxfer Group) (Funded by Luxfer Group Ltd.)

The grain refinement of twin roll cast aluminium alloys

Dr. M. Yun, Dr. M.E. Keeble, Professor J.D. Hunt, D. Bristow, Dr. R. Cook**

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. (*London and Scandinavian Metallurgical Co. Ltd.) (Funded by EPSRC and London and Scandinavian Metallurgical Co. Ltd.)

Residual stresses in Ti MMCs

Dr. S. Gungor, Professor C. Riuz*, Dr. J. Durodola**, Professor P. Bowen***, Professor B. Cantor*

Residual stresses in Ti MMCs are being investigated by modelling and measurements using novel moiré interferometry and slitting methods. The resulting creep, fatigue and damage mechanics are being measured and modelled to allow lifting of components. (*Department of Engineering; **Oxford Brookes; ***Birmingham University) (Funded by EPSRC, Rolls-Royce and DERA)

Grain refinement in Mg alloys

*Dr. B. Davies, Dr. K.A.Q. O'Reilly, Dr. P. Schumacher, J.F. King**

Metallic glasses, sedimentation and the entrained droplet technique are being used to investigate the mechanisms of grain refinement in model Mg alloys by Zr-containing particles. (*Luxfer Group) (Funded by Luxfer Group Ltd.)

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Heterogeneous nucleation in Al alloys is being investigated by using model glass-forming alloys. During rapid cooling of the glass forming melt, α -Al nucleates heterogeneously on added or quenched-in particles however growth is halted when the melt cools below the glass transition temperature. This enables the early stages of heterogeneous nucleation to be observed directly using transmission electron microscopy.

The micrograph shows a metastable hexagonal phase nucleating copious amounts of α -Al on its non-basal faces in a model Al-Si-Ni alloy.

Brian McKay and Dr. Pavel Cizek

E. Phase Transformations, Surfaces and Interfaces

I - PHASE TRANSFORMATIONS

Phase transformations of copper precipitates in ferritic matrices

*Dr. M.L. Jenkins, Professor G.D.W. Smith, Professor A.P. Sutton, A. Nicol, R.C. Doole, Dr. R. Monzen**

High-resolution electron microscopy (HREM) has shown that small coherent bcc copper precipitates in thermally-aged or irradiated iron alloys and some steels transform initially to a 9R structure by a martensitic mechanism, and then subsequently transform further to an fcc structure, probably by a diffusive mechanism. These transformation mechanisms are being elucidated by further HREM and theoretical studies. (*Kanazawa University, Japan) (Funded by EPSRC)

Heterogeneous nucleation in Al-Si alloys

B. McKay, Dr. P. Schumacher, Dr. K.A.Q. O'Reilly

Two novel techniques employing sedimentation and metallic glasses are being used to investigate the nucleation mechanisms operating when various grain refiner additions are made to Al-Si alloys. Refiner potency and the effects of alloying elements and processing conditions are also being evaluated. (Funded by EPSRC and in collaboration with London Scandinavian Metallurgical Company)

Structure and crystallisation kinetics of optical nanocomposites

Dr. A.K. Petford-Long, Dr. R. Serna, J.-P. Barnes, 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 British Council)

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.

Heterogeneous nucleation of 1xxx, 3xxx and 6xxx series Al alloys

Dr. C.M. Allen, Dr. K.A.Q. O'Reilly, Professor B. Cantor

DSC and TEM are being used to study the melting and subsequent heterogeneous nucleation of solidification of 1xxx, 3xxx and 6xxx series Al alloys in order to investigate phase selection and improve grain size control during DC casting. (Funded by EPSRC and Alcan International)

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)

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)

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. (Funded by Alcan International)

Modelling microstructure in multicomponent alloys

M. Shin, Professor J.D. Hunt

Diffusion based models will be used to predict microstructure in multicomponent alloys. The work will extend an existing model which treats two components. The model will predict the path of the liquid, microsegregation, the non equilibrium freezing range and will treat three and four phase reactions. The programme will initially use the NPL MTDATA database to provide thermodynamic data. (Funded by Alcan International and in collaboration with NPL)

A theoretical and experimental investigation of a novel scanning calorimeter

H. Dong, Professor J.D. Hunt

A novel calorimeter is being built to measure heat content as a function of temperature. the heat flow within the calorimeter will be modelled numerically to improve on the accuracy of the measurements. (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.

Microstructural modelling of model 7xxx series Al alloys

*Dr. A. Cerezo, Dr. K.A.Q. O'Reilly, Dr. J. Newman**

Alloy chemistry in model 7xxx series Al alloys is being investigated through a study of the fine-scale microstructure as a function of solidification and thermomechanical processing conditions. These studies will provide data for the development of thermodynamic models describing metastable phases, or the verification of existing models and databases. (*Luxfer Group) (Funded by Luxfer Group)

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

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

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. (Funded by EPSRC) (In collaboration with AEAT and INSS)

II - OXIDATION AND CORROSION

Corrosion of steel reinforcement in slag concretes

M. Holloway, Dr. J.M. Sykes

Alkali-activated slag concretes have potential for improving the durability of steel-reinforced structures because of low chloride permeability; this work examines how differences in structure and chemistry of the concretes influences chloride-induced corrosion of the steel reinforcement. (Funded by EPSRC and BNFL and in collaboration with Imperial College and Leeds University)

Pitting corrosion of stainless steel

Dr. J.M. Sykes

The work is investigating the fundamental significance of the critical pitting temperature and the mechanisms during the early development of pitting in chloride solutions.

Protection of metals by paint

Dr. J.M. Sykes

The mechanisms by which paint coatings fail during environmental exposure are being investigated using electrochemical methods and scanning acoustic microscopy. The barrier properties of the film and the role of inhibitive and other pigments is of particular interest.

III - SURFACE REACTIONS AND CATALYSIS

Controlled atmosphere analytical electron microscopy

*R.C. Doole, Dr. J.L. Hutchison, Professor M.J. Goringe**

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. (*Department of Engineering, University of Surrey)

One-dimensional crystal growth inside single-wall carbon nanotubes

Dr. J.L. Hutchison, Dr. J. Sloan, G. Brown, 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)

Controlled atmosphere TEM studies of mixed iron/antimony oxide ammoxidation catalysts

Dr. J.L. Hutchison, Professor M.J. Goringe, Professor M. Bowker***

Ammoxidation catalysts such as FeSbO₄ are being studied by high resolution, controlled atmosphere TEM. Particular emphasis is being placed upon determining the relative importance of the different Sb-bearing components of the system (as FeSbO₄, as a thin surface layer, and as macroscopic particles of oxide). (*Department of Engineering, University of Surrey; **Department of Chemistry, University of Reading) (Funded by EPSRC)

Catalytic atom probe

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 Omicron Surface Science Ltd.)

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High resolution image of $Nb_{16}W_{18}O_{94}$ taken in a JEOL 3000F field emission gun transmission electron microscope. If such images are obtained with a range of defocus values or beam tilts, the information within them can be combined digitally to achieve a resolution approaching the information limit of the microscope (below 0.1nm). (Work in collaboration with A.I. Kirkland, W.O. Saxton and R. Meyer of the University of Cambridge).

Dr. John Hutchison

F. Characterisation

I - SCANNING TUNNELLING AND ATOMIC FORCE MICROSCOPY

Semiconductor metallization in variable temperature STM/STS

*Dr. M.R. Castell, Professor G.A.D. Briggs, Dr. C. Norenberg, Dr D.R. Bowler**

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. (*University College, London)

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

*Dr. O.V. Kolosov, Dr. B. 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)

Growth and characterization of quantum silicide and nitride islands

Professor G.A.D. Briggs, Dr. M.R. Castell, Dr. S.D. Kenny, Dr. R.E. Rudd, Dr. C. Norenberg, 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.

Surfaces of oxides

*Dr. M.R. Castell, Professor G.A.D. Briggs, Professor A.P. Sutton, Dr. D.T. Goddard**

Low index surfaces of UO_2 and NiO are investigated by elevated temperature UHV-STM, LEED and AES. The influence of oxidation and reduction of these surfaces is studied. Covalent bonding in NiO can be revealed around defects on the NiO (001) surface which has far reaching consequences for the classification of this material. (*Research and Development, BNFL Springfield) (Funded by BNFL)

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

Dr. B. 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.

SPM of semiconductor quantum structures

Dr. O. Kolosov, Dr. B. Huey, Dr. N. Mason, Dr. M.R. Castell, Dr. C.D. Marsh, Dr. R.S. Williams**, Dr. T.I. Kamins**, Professor G.A.D. Briggs*

The growth and nanoscale mechanical properties of groups iii-v and group iv semiconductor buffer layers, superlattices and quantum dots are studied by various SPM techniques. (*Clarendon Laboratory, Department of Physics; **Hewlett-Packard Laboratories) (Funded by EPSRC)

Experimental development of heterodyne force microscopy

Dr. B. 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)

Direct measurement of interatomic potentials

Professor J.B. Pethica, Dr. P. Hoffmann, R. Grimble, 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. (*JRCAT, Tsukuba, Japan) (Funded by EPSRC and Paul Instrument Fund)

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. (*Inorganic Chemistry Laboratory; **Physical Chemistry Laboratory) (Funded by EPSRC)

New force microscopy techniques in ambient

S. Jeffery, Dr. P. Hoffmann, Professor J.B. Pethica

A new Polarisation Force Microscope has been constructed. It has very high resolution normal to the surface, allowing depth dependent characterisation. We are able to image dopants, trapped charge and insulator films on devices, and the local Kelvin null potential is being studied. PFM in liquid environment is planned.

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)

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

Dr. B. 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)

Room temperature manipulation of surface atoms

*Professor J.B. Pethica, Dr. P. Hoffmann, 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. (*Inorganic Chemistry Laboratory)

STM of oxides

Professor J.B. Pethica, Dr. C.E.J. Mitchell, Dr. R.G. Egdell*, Professor J.S. Foord***

A new STM and X-ray Photoelectron Spectroscopy (XPS) system is in use to study the topographical and electronic properties of bulk catalytic oxides, and also the early stages of the oxidation of metals. Surfaces under investigation include SnO₂, WOn and tungsten bronzes, ZnO. (*Inorganic Chemistry Laboratory; **Physical Chemistry Laboratory) (Funded by EPSRC)

Forces on single atoms in STM

*Professor J.B. Pethica, Dr. P. Hoffmann, S. Jeffery, 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. Comparison with atomically resolved AFM may lead to an understanding of the hitherto puzzling ability of STM to image low index metal surfaces. (*University of Tampere, Finland)

Atomic resolution AFM

Dr. P. Hoffmann, R. Grimble, S. Jeffery, 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. (Funded by EPSRC and Paul Instrument Fund)

Modelling AFM cantilevers

P. Boon, S. Jeffery, Professor J.B. Pethica

Finite element modelling is used to clarify the static and dynamic modes of practical AFM cantilevers, and help interpretation of experimental results. Of particular interest is the coupling between axes of applied forces and resulting displacements, and the coupling between modes in both resonant and non-resonant driven conditions.

II - ACOUSTIC MICROSCOPY

Nanoscale mechanics of fibre composites

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

Elastic and visco-elastic properties of carbon, ceramics and glass fiber composites and fiber-matrix interfaces are investigated with nanometre resolution by Ultrasonic Force Microscopy. (*RCC, Tokyo University)

Tip-surface mechanical interaction at ultrasonic frequencies

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

The absolute values of tip-surface elastic compliance and local elastic moduli measured by AFM in ambient environments are quantitatively evaluated using differential force ultrasonic force microscopy (UFM). (*Indian Institute of Physics, Bangalore)

Superlubricity under the ultrasonic vibration

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

The experimental and theoretical aspects of the phenomenon of decrease in friction coefficient between the AFM tip and sample under ultrasonic vibration are studied. (*Indian Institute of Physics, Bangalore)

Determination of hardness and modulus of thin films and coatings

*Dr. O.V. Kolosov, Professor G.A.D. Briggs, Professor A. Every**

We develop industrial standardization techniques for determination of hardness and elastic properties of thin sub-micrometer hard coatings by Brillouin spectroscopy. (*University of Witswatersrand, RSA) (Funded by EU)

III - FIELD-ION MICROSCOPY AND ATOM PROBE MICROANALYSIS

Atom probe microanalysis techniques

Dr. A. Cerezo, T.J. Godfrey, 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 Kindbrisk Ltd. and Omicron Surface Science Ltd.)

Atomic changes during strain ageing of steel wires

C. Hinchliffe, Dr. A. Cerezo, Professor G.D.W. Smith

The redistribution of carbon atoms which takes place during the annealing of cold-drawn steel wire is being studied by three-dimensional atom probe techniques. (In collaboration with British Steel)

Thermal ageing of steels

Dr. S. Hirosawa, 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)

Scanning atom probe

Dr. A. Cerezo, Dr. M. Huang, T.J. Godfrey, Professor G.D.W. Smith

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

Atom probe analysis of information storage materials

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 UHV evaporation and sputter deposition onto flat substrates and atom probe tips. The layer composition and interface nature are being studied using both conventional and position-sensitive 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 Monte Carlo simulations of the interdiffusion process. (*Seagate Technology) (Funded by Seagate Technology)

Solute distribution at grain boundaries in low-carbon steels

N. Maruyama, Dr. P.J. Warren, Professor G.D.W. Smith

A combination of TEM and 3DAP techniques are being used to study the atomic distribution of interstitial and substitutional solutes at grain boundaries in low carbon steels, as a function of boundary parameters and steel heat treatment. (Funded by Nippon Steel Corporation)

3D Reconstruction of atom probe data

O. Dimond, Dr. P.J. Warren, Dr. A. Cerezo*

A series of models for simulating atom probe data are being developed. These models will be used to aid interpretation of 3D atom probe data and develop better algorithms for 3D reconstruction. The experimental parameters limiting our ability to reconstruct the atomic lattice in 3D will be explored in detail. (*Kindbrisk Ltd.)(Funded by Kindbrisk Ltd.)

Early stages of precipitation in 6XXX automotive sheet

D. Vaumousse, Dr. P.J. Warren, 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)

IV - 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.

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)

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)

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)

Microstructure of diamond thin films

*Dr. J.L. Hutchison, Professor D. Shechtman**

Thin films of synthetic diamond, grown epitaxially on silicon, are being examined in both plan-view and cross-sectional specimens in order to elucidate the degree and nature of structural disorder present. (*Department of Materials Engineering, Technion, Haifa, Israel)

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 G.D.W. Smith

HREM is being used to study the structures 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.

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)

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, metal-ceramic interfaces, and superconductors. Recently new analysis methods have been developed at Oxford allowing elastic strains to be measured from the patterns. (The Royal Society)

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) is being installed for composition analysis and mapping of a wide variety of complex multicomponent metals, ceramics, composites, biomaterials and minerals. (*Department of Earth Sciences) (Funded by JREI)

TEM images of edge dislocations in slip planes parallel to the incident beam

Dr. S. Jiao, Professor Sir Peter Hirsch, Professor D.J.H. Cockayne*

Contrary to conventional wisdom, bright images of edge dislocations can be narrower than those of screw dislocations. This case arises when the slip plane is parallel to the incident beam, and $g \cdot b = 0$. Image profiles are being calculated and compared with experiment. The relative widths of bright field images can be used to distinguish edge dislocations lying on different slip planes. (*Argonne National Laboratory, Argonne IL, USA)

Quantum dot structures

Professor D.J.H. Cockayne, L. Xiaozhou, Dr. R. Leon**, Professor C. Jagadish****

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; **California Institute of Technology; ***Australian National University)

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)

Imaging dislocations in bulk materials by SEM channelling contrast

Dr. A.J. Wilkinson, Professor Sir Peter Hirsch

A novel technique has been developed at Oxford, whereby dislocations can be imaged near the surface of bulk specimens, the contrast arising from changes in the intensity of back scattered electrons near the defects. Individual dislocation lines can be observed to a depth of 100nm in bulk specimens using an SEM with a 30keV field emission gun. A further development has been to use an SEM with a conventional thermionic emission gun. Although this cannot resolve single dislocations clearly, groups of dislocations are readily seen to depths in excess of 1mm. (Funded by The Royal Society)

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)

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; (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)

Structure of amorphous materials

*Professor D.J.H. Cockayne, Dr. R. Dunin-Borkowski, 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. (*University of Sydney)

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)

Formation and Propagation of Subnano-Probes in the FEG(S)TEM

Dr. G. Möbus, Dr. R. Dunin-Borkowski, Professor J.M. Titchmarsh, Dr. J.L. Hutchison

The simulation of the optical beam formation for nanodiffraction and nanoanalysis will be performed for the new Oxford 3000F FEGTEM to be matched to experimental data. The proper control and focus selection for these beams is crucial to obtain optimum resolution. Beam propagation through crystalline samples will be examined with respect to judging resolution losses due to beam broadening and delocalised inelastic scattering. Extended calculations attempt to extrapolate properties of future high-performance TEMs with corrected optics.

Structure and stability of Cu-Al layered systems

*Dr. G. Möbus, Dr. B.J. Inkson, Dr. T. Wagner**

Thin films and multilayers of the Cu-Al system are examined by various electron microscopy techniques. Atomic structure, interdiffusion, and stability of the interface are studied at various temperatures. Analytical and high-resolution electron microscopy is applied in combination using the JEM3000F FEGTEM. (*MPI fuer Metallforschung Stuttgart, Germany)

Nanobeam analysis of strained layers with highest spatial resolution

Dr. G. Möbus, Dr. R. Dunin-Borkowski, Dr. J.L. Hutchison

Convergent beam electron diffraction is applied using the highly focused beam of the FEGTEM JEM-3000F to obtain local information on strain and composition of multilayered structures. The diffraction information is complemented by and compared to energy loss signals obtained with the same nanobeam. An automatised beam propagation mode to scan two-dimensional areas of interest on the specimen will be implemented.

Development of transmission electron microscopy for studies of crack tips

Professor J.M. Titchmarsh, A.N. Other

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 precipitation, intergranular segregation, lattice defects and alloy chemistry on crack nucleation and growth will be investigated by developing the techniques to prepare TEM specimens containing crack tips and characterising microstructures. Correlation between crack tip microstructure, applied stress and environmental parameters will be made. (In collaboration with Rolls Royce, AEAT and INSS)

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. R. Dunin-Borkowski

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 at 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. R. Dunin-Borkowski, Dr. J.L. Hutchison, 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)

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.)

Stability of precipitates under cascade-producing irradiation

Dr. M.L. Jenkins, Professor G.D.W. Smith, A. Nicol, R.C. Doole

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

Mechanisms of embrittlement in reactor pressure vessel steels

*Dr. M.L. Jenkins, Professor J.M. Titchmarsh, Professor P.B. Hirsch, Dr. R. Dunin-Borkowski, A. Nicol, 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) (Funded by EPSRC and in collaboration with BNFL Magnox Generation and Argonne National Laboratory)

VI - 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 1µm. 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 (<500nm) 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 (<30µm) 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 1µm 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 250µm 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 0.1µm diameter is running in parallel with collaborations in wide range of analytical projects.

A beam rocking system for angle resolved images of features in crystalline materials using ion channeling

D. de Kerckhove, Dr. G.W. Grime

Using an additional beam deflector the scanning system of the SPM can be modified to generate a beam deflection in angle instead of position which allows the system to be used to produce angle resolved channelling maps of crystalline materials, and can be used to explore lattice defects. Beam optical simulations were used to predict the optimum configuration of the scanning system to ensure that the beam position remains fixed on the sample during the beam rocking, and these were found to agree closely with experiment. Further work will concentrate on applying this system to crystallographic problems.

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, Dr. D.G. Fraser***

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 a glancing incidence) has been used to determine the concentration of metals reacted onto the surface of mineral crystals at sub-monolayer concentrations. The sensitivity for Zn on olivine surfaces was significantly better than using TRXRF with synchrotron radiation. (*University of Manchester Department of Earth Sciences; **University of Oxford Department of Earth Sciences) (Funded by NERC)

Deep ion beam lithography (DIBL) using MeV ion microbeams

D.de Kerckhove, Dr. G.W. Grime

The low scattering of MeV ions in solids means that the spatial resolution of the beam is maintained over a long range (typically 60 microns in silicon). We are investigating the potential of this property for fabricating high aspect ratio micro-structures in PMMA resist materials. Preliminary studies demonstrated that grooves 1 micron wide and 60 micron deep could be formed, and more recent work has produced miniature (100 microns diameter) gear wheels and turbines (with angled blades) in PMMA films.

Novel surfaces for metallic bone implants

Professor H. Plenk, Professor J. Helsen**, Professor S. Tschegg***, Dr. J.D. de Bruijn+, Dr. G.W. Grime, Professor C.B. Johansson++, Professor E. Schepers+++*

This collaboration is funded under the EC Biomed 2 programme and the aim is to investigate novel materials and fabrication methods for prostheses implanted directly into bone (e.g. dental implants). The role of the SPM in this collaboration is to investigate the bone/metal interface and measure by microPIXE any diffusion of metal ions and particles from the implant into the surrounding bone. (*Department of Bone and Biomaterials, University of Vienna A; **Department of Metallurgy and Materials Engineering, University of Leuven B; ***Department of Physics, University of Agriculture, Vienna A; +Biomaterials Research Group, University of Leiden NL; ++Department of Biomaterials, University of Göteborg S; +++Department of Prosthetic Dentistry and Biomaterials, Catholic University of Leuven B) (Funded by EC-BIOMED2)

Metals in hair from ancient bodies

*Dr. G.W. Grime, Dr. J. Powell**

Trace elements in hair from preserved bodies may give information concerning the lifestyle and state of health of individuals or ancient populations. Using the SPM it may be possible to distinguish surface contamination from metabolic uptake, and so provide more accurate assessments of lifetime trace element levels. We have analysed hair from the Neolithic ice body ("Ötzi") discovered recently in the Austrian Alps and found the presence of relatively high levels of As (comparable with those in a modern patient with low level chronic As poisoning) and high surface levels of Cu. These observations could be consistent with the theory that Ötzi was involved in copper metallurgy. In a separate investigation, hair from Napoleon Bonaparte are being investigated to shed more light on the theory that Napoleon died of arsenic poisoning. (*The Rayne Institute, St Thomas's Hospital, London)(Funded by The Rayne Institute and SERC)

Studies of lake sediment pore waters and particles

Professor W. Davison, Dr. G.W. Grime, Dr. G. Fones**

The cycling of Fe and Mn in lakes is in the form of a redox cycle in which the reduction phase is mediated by the decay of organic material in the upper layers of the sediment. This creates a source of metal ions in solution which diffuses back into the body of the lake. Thus the concentration gradient of metal ions of the sediment pore-water in the upper millimetres of the sediment is very steep and is crucial to the understanding of bio-geochemical cycling of metals. The SPM is being used in two studies of this system. 1) Using sampling probes of polyacrylamide gel films inserted vertically into the sediment water interface, the pore water content of the sediment can be measured with a spatial resolution of ~100 microns, an order of magnitude better than any previous technique. Various methods of preparing and deploying the probes are being investigated. 2) Sediment particles sampled at different depths in the lake are being analysed to determine their role in the cycle. In particular, RBS is being used to determine the oxidation state of iron oxide particles. (*University of Lancaster, Institute of Environmental and Biological Sciences) (Funded by NERC)

Development of a 0.1 micron Scanning Proton Microprobe beamline

Dr. G.W. Grime, D.de Kerckhove, Dr. E. Palsgard

A new beamline is under development which is planned to have a beam diameter of 0.1 micron 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 0.1 micron 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 - 30nm. The new beamline is expected to come on line in late 1998. (Funded by the Wellcome Trust)

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The molecule shown in the top figure is a repeat unit of a polyimide, known as PMDA-ODA. Polyimides are widely used in many industrial applications. Not much is known about the equilibrium structure of this polymer, especially the torsion about the imide-phenyl bond marked "X" in the top figure. Experimental estimates place this torsion angle between 0° and 60°. Our structure shown here is the result of the first fully ab initio-based geometry optimisation to be applied to PMDA-ODA. The method used a hybrid method called ONIOM which allows important interactions to be calculated using an accurate, time-consuming method (here it was MP2), while the rest of the molecule was treated using Hartree-Fock (HF) theory, which is very fast to evaluate and less accurate.

The bottom figure shows the energy of the PMDA-ODA fragment as a function of twisting the molecule about bond X. A torsion angle of 60° denotes a coplanar arrangement. The two barriers to rotation about this bond located at angles of 0° and 90° were determined through full transition-state searches using second derivatives of the energy. The solid line denotes the profile obtained using ONIOM with MP2. The other profiles show results from calculations based on density functional theory (DFT) and HF. We have shown in a separate calculation on a smaller molecule, malenil, that the ONIOM (MP2) method is the most reliable compared with full MP2 results. The bottom figure illustrates the deficiencies of both DFT and HF compared with the more reliable MP2-based results.

Dr Tiffany Walsh and Professor Adrian Sutton

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.

Effects of directional bonding on deformation and fracture of intermetallics

*Professor D.G. Pettifor, Dr. D. Nguyen Manh, Professor V. Vitek**

The influence of directional bonding on the deformation and fracture of intermetallics is being investigated at the atomistic level in order to understand why some intermetallics are brittle, whereas others are ductile. (*University of Pennsylvania)

CVD growth of diamond

*Professor D.G. Pettifor, Professor A.P. Sutton, Dr. I. Oleinik, Dr. J.E. Butler**

Analytic Bond-Order Potentials (BOPs) are being developed for the hydrocarbons in order to study the growth mechanisms of CVD diamond, in addition to performing more accurate atomistic simulations using Tight Binding and ab initio density functional theory. (*Naval Research Laboratory, Washington) (Funded by NRL, Washington)

Modelling the magneto-resistive 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 magneto-resistive 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)

Mapping of magnetization distributions in thin layered films

Dr. A.K. Petford-Long, Dr. P. Shang

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 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 at 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, Dr. 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)

Angularly-dependent potentials for atomistic simulations

*Professor D.G. Pettifor, Dr. D. Nguyen Manh, Dr. I. Oleinik, Professor M. Aoki**

A novel class of angularly-dependent potentials has recently been derived for covalently bonded systems within the Tight Binding approximation. These so called Bond-Order Potentials (BOPs) are currently being developed for hydrocarbons, semiconductors, transition metals, and intermetallics in order to perform realistic atomistic simulations of their properties. (*Gifu University, Japan) (Funded by British Council Collaborative Research Project)

Electron transport and electromigration in nanoscale conductors

Professor A.P. Sutton, Dr. T.N. Todorov, Dr. J.T. Hoekstra, Dr. J.M. van Ruitenbeek***

The electronic conductance of nanometre scale metallic wires has been calculated as they are pulled to fracture in a molecular dynamics simulation. These simulations have revealed the dramatic effect of mechanical instabilities and atomic rearrangements on the conductance. We are now considering the reverse question - the effect of the flow of current on the mechanical properties and stability of the wires. Starting from a tight-binding model, used to model both mechanical and electronic properties, we calculate the change in the density matrix caused by the flow of current, which then yields simultaneously the additional current induced forces on individual atoms and the local current flowing in each bond, allowing a direct comparison of the two. Separately, we wish to model local heating by the current. Our goal is to model current-induced mechanical effects such as electromigration and local heating, and to compare our results with experiments on real nanowires, carried out at Leiden. (*Dept. Physics, Queen's University Belfast; **Kammerlingh Onnes Laboratorium, Leiden) (Funded by EPSRC and Leverhulme Trust)

Dynamical Ising model simulations of phase separation

Dr. A. Cerezo, Dr. S. Hirose, 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 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 position-sensitive atom probe (PoSAP). (*AEA Technology, Harwell) (Funded by Rolls Royce Power Engineering)

Simulation of HREM images of metallic layered films

Dr. A.K. Petford-Long

The contrast observed in cross-sectional HREM images of metallic multilayer films is being modelled in order to predict the way in which it will change with interfacial abruptness between adjacent metal layers. In addition, modelling HREM images of multilayer films containing materials such as Co/Cu which show very poor differential contrast will enable the best experimental conditions to be predicted. (Funded by Hewlett-Packard Labs.)

Modelling near threshold fatigue crack propagation

H.-K. Lee, Dr. A.J. Wilkinson, Dr. S.G. Roberts

We are simulating the generation, interaction and motion of dislocations ahead of a crack tip during cyclic loading. The model predicts the occurrence of a threshold cyclic stress intensity for fatigue crack growth and tends to a Paris power law between crack growth rate and cyclic stress intensity at higher cyclic stress intensities. The model is being developed to more realistic mode I loading with crack tip blunting and microstructural features are being incorporated. (Funded by EPSRC and The Royal Society)

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. (*Fujitsu European Centre for Information Technology) (Funded by Fujitsu)

Modelling adhesion between polymers and inorganic substrates

*Professor A.P. Sutton, Dr. T.R. Walsh, Dr. C.G. Harkins**

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. (*Hewlett-Packard Labs, Palo Alto) (Funded by Hewlett-Packard Labs.)

CVD growth of carbon-nitride films

Professor E.G. Wang, Professor Lianmao Peng*, Dr. Gang Liu*, Dr. I. Oleinik, Professor D.G. Pettifor*

A variable time-step kinetic Monte Carlo model will be developed to model the CVD growth of carbon-nitride films in conjunction with an experimental study. (*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*, 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. S.L. Dudarev, 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. (*UKAEA Fusion, Culham Science Centre; **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

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

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. (Funded by EPSRC)

Fundamentals of brittle-ductile transitions

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

Theoretical and modelling studies of crack tip - dislocation interactions which control brittle-ductile transitions in metals, intermetallics and ceramics. The plastic zones around a crack are modelled by computer simulation of dislocation arrays around the crack tip. The modelling is being applied to the brittle transition in steels. (Funded by EPSRC and AEAT)

A simple tight binding model for noble metals

Professor A.P. Sutton, Dr. J. Hoekstra, M. Cawkwell

A simple 1-s tight binding model for noble metals is being tested, with particular regard to the correct prediction of the f.c.c. ground state structure, the elastic constants and the vacancy formation energy. This is probably the simplest electronic structure based model that has ever been devised for any metal. (Funded by Leverhulme Trust)

Concurrent multi-scale simulation of microsystems

Dr. R.E. Rudd

Concurrent multi-scale simulations are being developed for fracture and dynamical microsystems, classic examples of systems with multiple length scales. These simulations balance accuracy and efficiency by partitioning systems into domains characterised by Angstrom, nanometre and micron length scales. Each domain is handled with a different methodology--electronic structure, atomistics and continuum mechanics--and the domains are joined together seamlessly via handshaking interactions. The multi-scale model is able to treat the breaking of quantum-mechanical bonds at a crack tip simultaneously with the propagation of elastic strain fields that extend for more than a micron from the crack tip. (Funded by DARPA and DoD HPCMO, USA)

Atomistic simulation of the dynamics of MEMS

*Dr. R.E. Rudd, Dr. J.Q. Broughton**

Atomistic modelling is employed to study the effect of surface processes on the dynamics of sub-micron Micro-Electro-Mechanical Systems (MEMS). This research is initially focusing on MEMS resonators, in which oscillations of the resonators are simulated in order to predict anomalous frequency shifts and dissipation due to atomistic processes. Results of the atomistic simulations are used to build new constitutive relations suitable for continuum models of the sub-micron systems. (*Yale University, USA) (Funded by DARPA and DoD HPCMO, USA)

Refinement of structures by microscopy, diffraction and atomistic modelling

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

Techniques will be further developed for refining structural models of amorphous and crystalline materials at the atomic level by combining HREM and electron diffraction data with atomistic modelling techniques. (*University of Sydney)

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The caption for this picture should be: Fragment of copper smelting slag from Pentwyn, Great Orme, Llandudno. The fragment comes from a test smelt of Middle Bronze Age date (mid 2nd millennium BC) and is part of the first find of dated copper smelting slag from the British Bronze Age. The material is currently being evaluated by the Materials Science-Based Archaeology Group.

Chris Salter

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, 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. (In collaboration with The Royal Armouries, Leeds)

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).

Precipitation of copper in silver alloys

*Dr. J.P. Northover, J. Hirx**

The discontinuous precipitation of copper at grain boundaries from supersaturated solid solution at room temperature in wrought and annealed silver alloys with 2-10% copper has been advanced as an indication of age. This project will make the first transmission electron microscope studies of the morphology and structure of the precipitates, determine the length, if any, of an incubation period, and find the conditions under which precipitation changes from discontinuous to continuous. The possibility of accelerating the discontinuous precipitation by annealing at intermediate temperatures will also be explored. (*Conservation Section, Los Angeles County Museum of Art)

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)

Application of the scanning proton microprobe to the analysis of Egyptian 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 Egyptian 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.

Non-ferrous and precious metallurgy in the European Iron Age

Dr. J.P. Northover, P. Nagy, P. Ramsler**, 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)

Anglo-Saxon Ferrous Technology

C.J. Salter, G. Hey, 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)

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

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

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

Study of possible Bronze Age copper smelting debris from the Great Orme, Gwynedd, Wales

*C.J. Salter, Dr. J.P. Northover, S. Jones**

Although there is extensive evidence of Bronze Age mining activity in Britain, as yet no evidence of prehistoric copper smelting has been discovered on the British mainland. A small quantity of slag-like material from contexts dated to circa 1580 BC are being studied to determine its nature and mode of origin. This will include experimental reproduction. (*Gwynedd Archaeological Trust)

Effects of conservation techniques in bronze

Dr. J.P. Northover, N. Norman, M. Sahlstedt***

A combination of optical and scanning electron microscopy, electron microprobe analysis and PIXE/RBS spectrometry will be used to compare the effects of different conservation methods of a group of Bronze Age tools and weapons. Particular attention will be paid to the preservation of surface detail during cleaning and treatment, and to the distribution of inhibiting species in the corrosion and patina after treatment. (*Department of Antiquities, Ashmolean Museum; **Conservation Institute, Gothenburg University)

The development of rail steels

*Dr. J.P. Northover, F. Horbury, D. Wright**

The collections of the National Railway Museum will be utilised to study the development of materials for rails. The collection extends from cast iron tramplates at the end of the 18th century through wrought iron to early Bessemer steel to eutectoid and alloy steels. Metallography and microanalysis will be used to characterise the irons and steels and the results will be compared with the documentary history of the subject. The project is designed in particular to examine the impact of steel and understand the problems associated with its introduction in railway use. (*National Railway Museum, York)

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