



Research in Progress  
2002 - 2003



Department of Materials



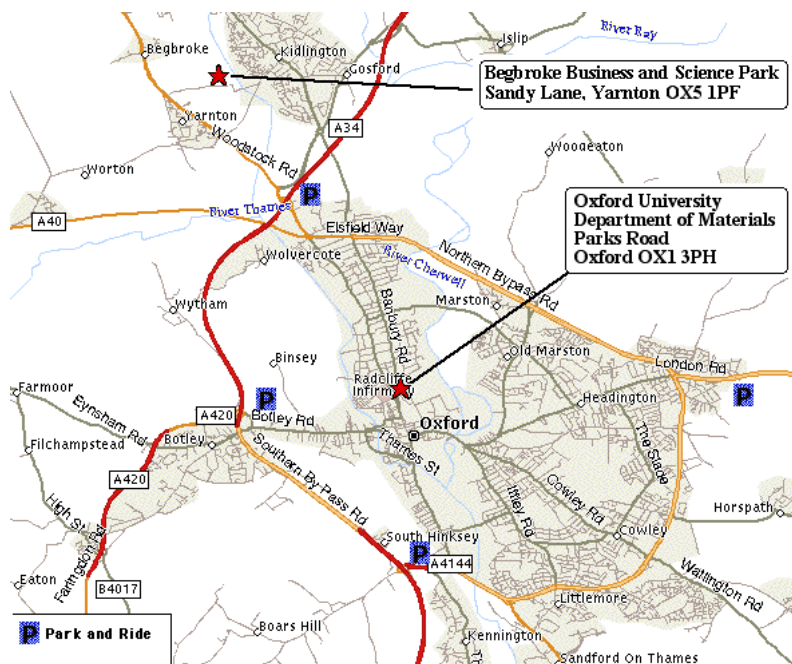


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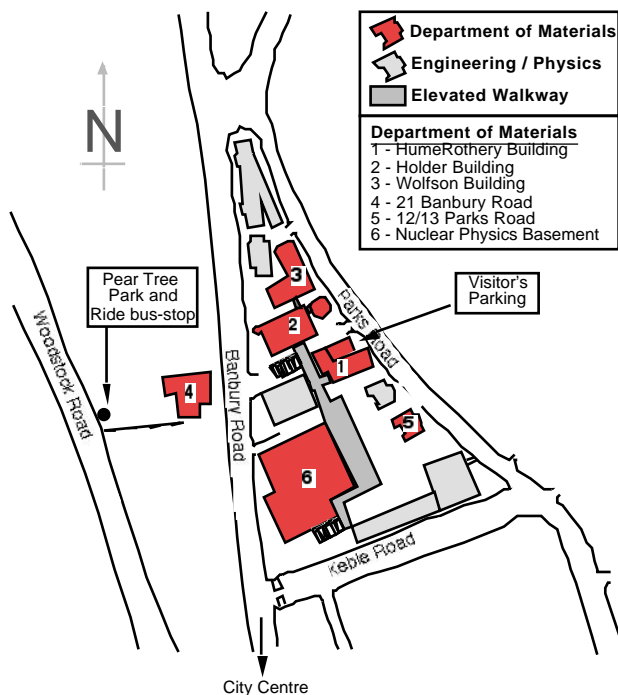
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## Department of Materials

## University of Oxford

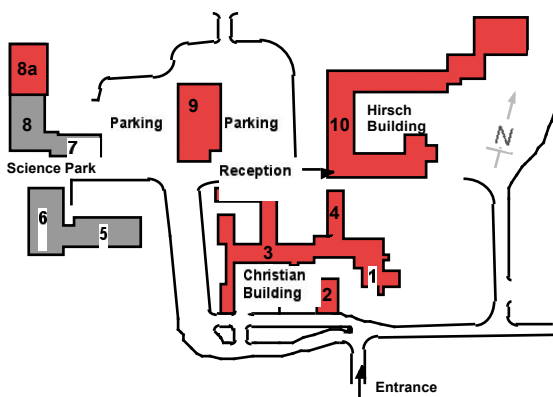


### Department of Materials Keble Road Triangle



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

Welcome to the Department of Materials at Oxford University. Our objectives are to produce world class graduate materials scientists and engineers, and to conduct world class research into the manufacture, structure, properties and applications of materials, for the benefit of the UK and world community. We were awarded the highest grading for research and 23 out of 24 in the government's most recent assessment exercises, and we continue to make outstanding progress in the pursuit of our objectives.

Major advances over the last four years include:

1. 1 Three new Professorships, in nanomaterials (Andrew Briggs), electron microscopy (David Cockayne) and structural integrity (John Titchmarsh);
2. 2 Four elections to Fellowships of the Royal Society (David Cockayne, John Pethica, Brian Eyre and John Hunt) and two elections to the Royal Academy of Engineering (Richard Brook and Brian Cantor);
3. Awards and honours to members of the Department, including the Royal Society Armourers and Brasiers Award (David Pettifor, John Hunt), the Royal Society Hughes Medal and the IofP/SFP Holweck Medal and Prize (John Pethica), the Institute of Materials Platinum Medal (John Martin, Brian Cantor), the Beilby Medal and Prize (Alfred Cerezo), the Pfeil Award (Richard Todd), Metrology for World Class Manufacturing Awards (Andrew Briggs, Oleg Kolosov, John Hunt), and election to the US National Academy of Engineering and award of the Heyn-Denkmuze prize of the German Materials Society (Sir Peter Hirsch). Richard Brook received a knighthood, and was appointed Director of the Leverhulme Trust, Andrew Briggs was appointed as the Director of a new Quantum Information Processing Interdisciplinary Research Center, John Hutchison was elected President of the Royal Microscopical Society and David Cockayne was elected President of the International Federation of Societies of Microscopy (2003-6).
4. Four promotions to personal professorships (Adrian Sutton, Amanda Petford-Long, Alfred Cerezo and Andrew Briggs) and eight promotions to readerships (Alfred Cerezo, Patrick Grant, Chris Grovener, John Hutchison, Mike Jenkins, Amanda Petford-Long, Steve Roberts and John Sykes);
5. Over £8m from the Joint Infrastructure Fund, to purchase cutting edge equipment for atomically engineered, nanoscale materials processing and analysis
6. The launch of the new £22m Begbroke site, which greatly expands the Department's space, and sets up a unique combination of industry-linked materials research and spin-out science park;
7. The establishment of a Faraday Partnership in aerospace and automotive materials; and
8. The award of a £3.4m DTi Foresight Link grant for research on nanoelectronics and quantum computation.

The Department was founded by Professor Hume-Rothery in 1956. At present, it consists of 24 academics, 16 senior researchers, 51 postdoctoral researchers, 38 technicians and administrative staff, 33 academic visitors, 92 research students and 101 undergraduates. The Department is part of an integrated Division of Mathematical and Physical Sciences at Oxford, which includes physics, chemistry computing and engineering departments, providing an ideal environment for interdisciplinary teaching and research. Fundamental developments in the physics and chemistry of materials can take place directly alongside applications in manufacturing processes and engineering design.

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

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

October 2002  
Oxford

## Members of Department

### Professors

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

### Readers

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

### Lecturers

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

### Administration

Dr. R.M. Plummer	<i>Administrator</i>
Mrs. D. Faulkner	<i>Deputy Administrator (Finance)</i>
Vacant	<i>Deputy Administrator (Academic)</i>

## Senior Research Fellows

Dr. R. Ball	Wolfson Industrial Fellow	Dr. J.W. Martin	OCAMAC Senior Fellow
Dr. S. Benjamin	Royal Society Research Fellow	Dr. C. Nörenberg	RS Dorothy Hodgekin Fellow
Dr R. Bhatti	Senior Visiting Fellow (QinetiQ)	Dr. O.V. Salata	OCAMAC Industrial Fellow
Dr. G.R. Booker	OCAMAC Senior Fellow	Dr. C.B. Scruby	Wolfson Industrial Fellow
Dr. M.R. Castell	Royal Society Research Fellow	Dr. J. Sloan	Royal Society Research Fellow
Dr. R. Falster	OCAMAC Senior Fellow	Dr. I.C. Stone	Senior Research Fellow
Dr. B. Gilmore	Senior Visiting Fellow	Dr. G. Taylor	Senior Research Fellow
Prof. R. Howson	Senior Visiting Fellow	Dr. D. Vesely	OCAMAC Senior Fellow
Dr. D. Imeson	Senior Visiting Fellow (DSTL)	Dr. A.J. Wilkinson	Royal Society Research Fellow

## Research Fellows

Dr. R.J. Baxter	Dr. S. Hoile	Dr. J. Mi
Dr. M.S. Bobji	Dr. C. Johnston	Dr. Duc Nguyen Manh
Dr. V. Burlakov	Dr. J-H. Kang	Dr. J.H.G. Owen
Dr. M J Carey	Dr. K.R. Kirov	Dr. D. Ozkaya
Dr. A. Cock	Mr. A.N. Khlobystov	Dr. I.G. Palmer
Dr. A. Crossley	Dr. A.I. Kirkland	Dr. D. Pankhurst
Mr. F. Cullen	Dr. K. Kohary	Mrs S. Panteny
Dr. Z. Djuric	Dr. R. Langford	Dr. K. Porfyraakis
Dr. M. Döblinger	Dr. P. Leigh	Dr. B. Reddy
Dr. H-B. Dong	Dr. S.M. Lee	Mr. C.J. Salter
Mr. R.C. Doole	Dr. J. Leopoldes	Dr. G. Sha
Dr. A. Dupuis	Dr. S. Lorenz	Dr. M. Tomut
Mr. T.J. Godfrey	Dr. B. Lovett	Dr. B. Warot
Dr. R. Hansen	Mr. S. Lozano-Perez	Dr. P.J. Warren
Dr. B.M. Henry	Dr. Y-Q. Ma	Dr. S.J. Wilkins
Dr. C.J.D. Hetherington	Dr. K. Mallik	Dr. H. Wu
Dr. S.C. Hogg	Dr. C.D. Marsh	Dr. H-L. Zhang

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## D.Phil and MSc. Research Students

Abraham, M.H. (self-supporting)  
Ahmed, S. (CASE: Corus)  
Allsop, N. (EPSRC / St. Annes Scholarship)  
Austwick, M.R. (EPSRC)  
Bagot, P. (EPSRC)  
Barnes, J-P. (EPSRC)  
Bernardo, C. (self-supporting)  
Briceno-Gomez, M. (Qinetiq)  
Britz, D. (EPSRC Foresight Link)  
Bromwich, T. (EPSRC DTA)  
Brown, G. (CASE: Colebrand Ltd.)  
Campbell, P.J.D. (CASE: BNFL)  
Carter, R. (EPSRC)  
Castro Diaz, L. (Regenesys / Linacre)  
Chadd, G. (Crown Cork & Seal)  
Chen, X. (self-supporting)  
Choi, Y-S. (EPSRC)  
Coates, M. (EPSRC)  
Cockfield, T. (CASE: Alcan)  
Dark, C.J. (EPSRC DTA)  
Davidson, I. (CASE: Alcoa Extrusions)  
Davin, L. (EPSRC)  
DeMorais, A. (Nordiko Ltd)  
Di Maio, D. (Hardide)  
Doherty, M.J. (EPSRC)  
Eggeman, A. (EPSRC DTA + CASE: Johnson Matthey)  
Galano, M. (EU/Korea/Clarendon/ORS)  
Giannattasio, A. (MEMC Ltd.)  
Gilberti, L. (EPSRC)  
Gomez-Morilla, I. (BNSC)  
Gotora, D. (Rhodes)  
Gunlycke, D. (EPSRC Foresight Link)  
Hedges, M.K. (EPSRC)  
Hinchliffe, C. (CASE: Rolls-Royce)  
Howells, D. (CASE: Dupont)  
Hudson, T. (AEA / Linacre)  
Ito, F.  
Kawata, K. (Toppan Printing Co.)  
Kim, H.S. (self-supporting)  
Kim, K-B. (self-supporting)  
King, O. (EPSRC)  
Kurum, E. (EPSRC)  
Lambourne, A. (Department)  
Lang, C. (EPSRC)  
Langham, C. (Motorola)  
Leigh, D. (EPSRC Foresight Link)  
Manson-Whitton, C.D.J. (Royal Commission for the Exhibition of 1851 Scholarship / Luxfer Ltd.)  
Mason, D. (EPSRC / Applied Materials Linacre Scholar)  
Mathieson, D. (OPSYS)  
Morgan, D.L. (EPSRC)  
Morley, G. (EPSRC Foresight Link)  
Morton, J. (EPSRC DTA / NEDO)  
Nazir, A. (EPSRC)  
Nicholls, R. (EPSRC DTA, St Catherine's Scholarship)  
Nzula, M. (visiting student, Sainsbury Scholarship)  
Okayasu, T. (Oji Paper Co.)  
Oliver, R.A. (EPSRC)  
Owen, N.W. (EPSRC)  
Pak, S.J. (Self-supporting)  
Park, S-B. (self-supporting)  
Ramanujan, C.S.  
Rayment, T. (EPSRC / St. Cross Scholarship)  
Russell-Stevens, M.J. (EPSRC)  
Sachlos, E. (St. Peter's College)  
Saran, M. (ORS/Chevening/self-supporting)  
Saunders, S. (CASE: National Physical Laboratory)  
Scipioni, R. (Self / EPSRC Foresight Link)  
Shapiro, I. (EPSRC DTA)  
Shinotsuka, K. (self-supporting)  
Speller, S. (EPSRC)  
Srimanosaowapak, S. (Thai Gov.)  
Stowe, D.J. (EPSRC)  
Taylor, R.N. (CASE: Nanox)  
Todorovic, M. (Scattered Scholarship)  
Vaumousse, D. (CASE: Alcan International Ltd.)  
Wain, N. (EPSRC)  
Walpole, A. (EPSRC DTA)  
Wang, H. (Clarendon/ORS)  
Waring, M. (EPSRC DTA)  
Whiteley, R.M. (EPSRC)  
Whyte, E. (CASE:Corus)  
Wilkinson, S. (EPSRC / Guy Newton Wolfson Scholar)  
Xie, Z. (Clarendon /ORS)  
Xu, J. (self-supporting)  
Zhang, L. (ORS)  
Zhou, Dr Z. (UKAEA)  
Zhu, M. (K.C.Wong / ORS)

## Part II Students (4<sup>th</sup> Year Undergraduates)

### Materials Science

Colvin, D.R.  
Goodsir, L.  
Grennan-Heaven, N.  
Griffiths, S.T.  
Imrie, J.W.  
Joseph, T.D.B.

Nicholson, W.  
Scruby, L.A.  
Smart, K.  
Vasa, C.E.I.  
Vaughan, T.D.  
Waller, J.H.

### Materials, Economics and Management

Dickson, A.R.  
Evans, P.I.  
Henry, S.C.  
Kirk, D.J.  
Newell, D.T.  
Ogle, C.J.  
Wilkinson, E.K.

### Engineering and Science of Materials

Chung, C.  
D'Arcy, M.J.  
Kemp, E.J.  
Kirton-Vaughan, A.  
Mallinson, I.P.  
Sarsfield, H.R.

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



## **Visiting Academics (2001-2002)**

Dr F E Audebert, University of Buenos Aires, Argentina  
Prof V Baranauskas, Campinas State University, Brazil  
Prof J C Bilello, University of Michigan, USA  
Ms C Bishop (graduate student), MIT, USA  
Dr P Butler, Crown Cork & Seal Co Inc, UK  
Mr R H Chauke (graduate student), University of the North,  
South Africa  
Dr D Crespo, Catalan Polytechnic University, Spain  
Dr M J Daniels, University of Michigan, USA  
Dr A J Doyle, Doyle & Tratt Products Ltd, UK  
Prof B L Eyre, Central Laboratory of the Research Councils  
Dr R Falster, MEMC Electronic Materials, Italy  
Prof M W Finnis, Queen's University, Belfast  
Mrs S Gillis (graduate student), University of Minnesota  
Dr B J J Gilmour, University of Oxford  
Prof E Gruenbaum, University of Tel-Aviv, Israel  
Dr S Gubenko, National Metallurgical Academy of Ukraine  
Miss R E Harper, Accentus, UK  
Dr K Hrytsenko, Ukrainian National Academy of Sciences  
Dr B Huey, University of Oxford  
Miss M Huhtala (graduate student), Helsinki University of  
Technology, Finland  
Dr R Iqbal, Microsharp Corporation, UK  
Prof H S Kim, Chungnam National University, S Korea  
Dr S H Kim, Yonsei University, S Korea  
Prof N A Kisilev, Russian Academy of Sciences  
Dr D L Larson, Seagate Technology, USA  
Dr Q L Li, Chinese University of Hong Kong  
Prof B-G Liu, Chinese Academy of Sciences, P R China  
Dr G Lloyd, CVT Ltd, UK  
Dr N Marks, University of Sydney, Australia  
Dr M Martín-Fernández, University of Oxford  
Dr M Matsukawa, Doshisha University, Japan  
Prof T Mori, Rutherford Appleton Laboratory, UK  
Dr S Mukhopadhyay, Inter-Universities Consortium for DAE  
Facilities, India  
Miss N E Munoz (graduate student), University of Minnesota  
Dr N Mustapha, Opsys Ltd, UK  
Dr S Myhra, Griffith University, Australia  
Prof A H W Ngan, University of Hong Kong  
Prof H Ohsawa, Hosei University, Japan  
Dr H Ö Özer, Trinity College Dublin, Republic of Ireland  
Dr D Ozkaya, University of Oxford  
Dr I G Palmer, Oxford [no affiliation]  
Prof C J Peel, QinetiQ Ltd  
Prof L-M Peng, Chinese Academy of Sciences, P R China  
Prof J B Pethica (University Visiting Professor), Trinity  
College Dublin, Republic of Ireland  
Prof A P V Priftaj, Polytechnic University of Tirana, Albania  
Dr A N Safonov, Opsys Ltd, UK  
Dr K L Sahoo, National Metallurgical Laboratory, India  
Dr U Schönberger, Max-Planck Institute for Solid State  
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Dr S Senkader, University of Exeter, UK  
Dr M S Shchepinov, Russia [affiliation unknown]  
Mr N Skukan (technician), Ruder Boskovic Institute, Croatia  
Dr C Sofield, Oxford [no affiliation]  
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Mr M Ushirozawa, Japan Broadcasting Corporation  
Dr T V Visart de Bocarmé, Free University of Brussels  
Mr S von Alftan (graduate student), Helsinki University of  
Technology, Finland  
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Prof J V Wood, Central Laboratory of the Research Councils  
Prof H Yang, Wuhan University of Technology, P R China  
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Professor B.L. Eyre, CBE, FREng, Chairman, Central Laboratory for the Research Councils  
Mr. R. Malthouse, Cookson Group  
Dr. C.C. Morehouse, Director, Information Storage Technology Lab, Hewlett-Packard USA (Committee Chairman)  
Dr. J. Patterson, British Nuclear Fuels  
Professor C.J. Peel, Director, Technology (Strategy), FST, QinetiQ Ltd  
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Dr. K.A.Q. O'Reilly, Department of Materials, University of Oxford  
Mr. C. Purcell  
Professor G.D.W. Smith, FRS, Department of Materials, University of Oxford

## Research Sponsors

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

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Helsinki University of Technology	Rolls-Royce Power Engineering
Hardide	Royal Academy of Engineering
Health and Safety Executive	Royal Commission for the Exhibition of 1851
Hewlett-Packard	Scatcherd Scholarship, Merton College
Higher Education Funding Council for England	Seagate Technology Ltd
Hitachi Europe	Sulzer Metco
INSS	Thai Government
Institute of Materials	The Royal Society
Ironmongers Company	Toppan Printing Company
Japanese Research Council	UKAEA
JEOL UK Ltd	Wellcome Trust

## Profiles of Academic Staff



**Dr. Hazel Assender**  
*Linacre College*

**Lecturer in Materials**

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



**Dr. Simon Benjamin**  
*Exeter College*

**Royal Society University Research Fellow**

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



**Dr. Roger Booker**  
*Wolfson College*

**Emeritus Reader in Electronic Materials**  
**OCAMAC Senior Fellow**

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



**Professor Andrew Briggs**  
*Wolfson College*

**Professor of Materials**

Director of Quantum Information Processing Interdisciplinary Research Collaboration.

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



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

**Professor of Materials**

Processing and properties of ceramic materials.

[ Currently Director of the Leverhulme Trust]



**Dr. David Bucknall**

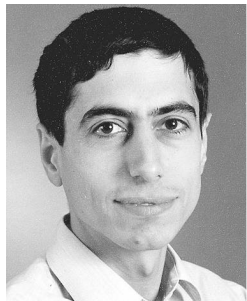
**Lecturer in Materials**

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



**Dr. Martin Castell CPhys**      **Royal Society University Research Fellow**  
*Wolfson College*

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



**Professor. Alfred Cerezo**  
*Wolfson College*

**Professor of Materials**

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

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



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

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

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



**Dr. Jan Czernuszka**  
*Trinity College*

**Lecturer in Materials**

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

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



**Professor Brian Eyre CBE FEng. FRS**      **Visiting Professor**  
*Wolfson College*      **Wolfson College Industrial Fellow**

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

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



**Dr. Patrick Grant**  
*Linacre College*

**Reader in Materials Processing**  
**Director of OCAMAC**  
**Director of Faraday Partnership**

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



**Dr. Chris Grovenor**  
*St Anne's College*

**Reader in Materials**  
**Deputy Head of Department**

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



**Professor Sir Peter Hirsch FRS, FIM**  
*St Edmund Hall*

**Emeritus Professor**

Electron microscopy of defects in crystals and modelling mechanical properties of crystalline materials in terms of dislocation processes. Recent interests include modelling the brittle-ductile transition and plastic properties of intermetallics.

- Royal Society : Hughes Medal 1973 and Royal Medal, 1977.
- Metals Society Platinum Medal 1976
- Wolf Prize in Physics, 1983
- Acta Metallurgica Gold Medal, 1997



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

**Emeritus Professor**

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

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



**Dr. John Hutchison**  
*Wolfson College*

**Reader in Materials**

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

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



**Dr. Mike Jenkins**  
*Jesus College*

**Reader in Materials**  
**Director of Electron Microscope Facilities**

Radiation damage, transmission electron microscopy, phase stability under irradiation. Recent work has focused on fundamental mechanisms of radiation damage, especially displacement cascade processes, mechanisms of embrittlement of pressure vessel steels, and quantitative imaging of defects.



**Dr. John Martin**  
*St Catherine's College*

**Emeritus Reader**  
**OCAMAC Senior Fellow**

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

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



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

Growth of quantum nitride nanostructures (InGaN, AlGaIn) by molecular beam epitaxy (MBE) and in-situ surface characterisation by elevated-temperature scanning tunnelling microscopy (STM) and electron diffraction to investigate nucleation and elucidate growth modes. Study of size and shape distribution of quantum dots to develop a nanostructure diagram as a function of codeposition and growth parameters.



**Dr. Peter Northover**  
*St Catherine's College*

**Lecturer in Materials**  
**Practical Class Organiser**

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



**Dr. Keyna O'Reilly**  
*The Queen's College*

**Lecturer in Materials**

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

**Professor Chris Peel**

**Visiting Professor**

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



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

**Professor of Materials**

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

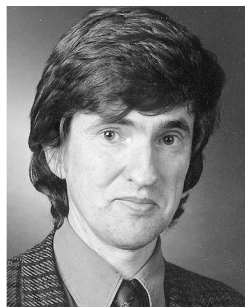


**Professor John Pethica FRS**  
*St Cross College*

**Visiting Professor**

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

- Hughes Medal, The Royal Society, 2001.
- Rosenhain Medal and Prize, Institute of Materials, 1997.
- Sabbatical Chair, Sony corporation R&D, Japan, 1993-4.



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

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

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



**Dr. Rosetta Plummer**  
*St Edmund Hall*

**Department Administrator**

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



**Dr. Steve Roberts**  
*St Cross College*

**Reader in Materials**

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



**Dr. Oleg Salata**

**OCAMAC Senior Research Fellow**

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



**Dr. Jeremy Sloan**  
*Wolfson College*

**Royal Society University Research Fellow**  
**(joint with Department of Chemistry)**

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



**Professor George Smith FRS**  
*Trinity College*

**Professor of Materials  
Head of Department**

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

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



**Dr. Ian Stone**

**Senior Research Fellow**

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



**Professor Adrian Sutton FInstP, FIM**      **Professor of Materials Science**  
*Linacre College*

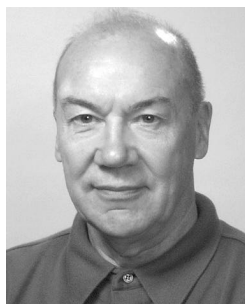
Modelling of materials at the atomic and microstructural levels. Adhesion of polymers to inorganic substrates. Mechanical, thermal and electrical properties of metallic nanocontacts. Electromigration. Long-range elastic interactions and microstructural evolution due to diffusional phase transformations.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



**Dr. John Sykes**  
*Mansfield College*

**Reader in Materials**

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



**Dr. Glyn Taylor**  
*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  $\gamma$ -TiAl and various B2 compounds. Relating yield stress and strength to the properties of dislocations. Measuring elastic constants.



**Professor John Titchmarsh**  
*St Anne's College*

**RAE Research Professorship in  
Microanalysis and Structural Integrity**

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





**Dr. Richard Todd**  
*St Catherine's College*

**Lecturer in Materials**

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

- Pfeil Award, Institute of Materials, 2001.



**Dr. Drahosh Vesely**  
*Wolfson College*

**OCAMAC Senior Fellow**

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



**Professor Mike Whelan**  
*Linacre College*

**Emeritus Professor**

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

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



**Dr. Angus Wilkinson**  
*Corpus Christi College*

**Royal Society University Research Fellow**  
**Lecturer in Materials**

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



**Dr. Peter Wilshaw**  
*St Anne's College*

**Lecturer in Materials**

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



**Professor John Wood**

**Visiting Professor**  
**Wolfson College Industrial Fellow**

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

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

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## ***A. Structure and Mechanical Properties of Metals***

### **I - MECHANICAL PROPERTIES OF STRONG SOLIDS, METALS AND ALLOYS**

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

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

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

#### ***Physical properties of Li-Mg alloys***

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

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

#### ***Measurement and development of residual stresses in coatings***

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

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

#### ***Fundamentals of cyclic deformation and fatigue crack initiation***

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

The evolution of dislocation microstructures produced during cyclic deformation is being examined using electron channelling contrast imaging, a novel SEM technique. The objective is to understand the reasons for dislocation patterning and subsequent strain localisation leading to the initiation and early growth of fatigue cracks. Recent work concerns Si fatigued at elevated temperatures. (\*Ecole des Mines, Nancy, France)(Funded by The Royal Society)

#### ***Nanoscale deformation of materials quantified by TEM nanoindentation***

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

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

#### ***Carbide cracking and the brittle-ductile transition in ferritic steels***

*M. Coates, Dr. A.J. Wilkinson, 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)

**Microstructure-property relationships in commercial superplastic 7475-aluminium alloys**

S. Griffiths, Dr. R.I. Todd, Dr. N. Ridley\*

The microstructural features controlling flow stress during superplastic forming of commercial 7475-Al alloys are being investigated. The microstructures and mechanical properties of contrasting materials are being compared. (\*University of Manchester) (Collaborators: BAE Systems)

**Development of corrosion resistant high strength ferritic steels**

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

High strength ferritic steels are prone to stress corrosion cracking. This project aims to improve cracking resistance by modifying the composition of Ni-Mo-containing ferritic steel by selected elemental additions. Alloys will be made by melt spinning and mechanical and corrosion properties optimised by

systematic variation of heat treatment and microstructural characterisation. (\*QinetiQ)

**Advanced stress analysis by laboratory X-ray diffraction**

Dr. P.S. Grant, Dr. A. Korsunsky\*, Professor D. Nowell\*

A state-of-the-art x-ray diffraction facility with the capability to undertake XRD during in-situ straining of specimens has been installed in the Department of Engineering Science and is being used in investigations of residual stresses and stress evolution in a range of model and engineering materials. (In collaboration with \*Department of Engineering Science and funded by EPSRC).

## II – INTERMETALLICS

**Mechanical properties of CoTi based alloy single crystals**

L. Zhang, Dr. M.L. Jenkins, Dr. G. Taylor

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

**Mechanical properties of lamellar TiAl and effects of purity and composition**

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

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

**3D microstructural characterisation of intermetallics**

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

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

**Deformation of  $\gamma$ -TiAl single crystals with [001] orientation**

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

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

***Simulation of weak-beam images of defects in  $\gamma$ -TiAl***

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

Weak beam images of  $1/2[112]$  edge dislocations in  $\gamma$ -TiAl are being simulated using the CUFOUR programme with a view to distinguishing between possible alternative structures of these defects. A model has been developed to explain the locked nature of these defects.

***The growth and deformation of TiAl<sub>3</sub> single crystals***

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

Transition metal additions to TiAl<sub>3</sub> are being made to stabilise the cubic structure. Single crystals will be grown and used for deformation studies. (\*Suranaree University of Technology, Thailand)

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

*S.J. Pak, 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. RuAl has a high melting point and the vapour pressure of Al when the alloy is molten is sufficiently high to make the growth of single crystals difficult. A floating-zone crystal growth apparatus has been constructed for operation at above ambient pressure in an attempt to grow good quality crystals of RuAl and other B2 intermetallic compounds.

***Formation of APB tubes in  $\gamma$ -TiAl***

*Professor Sir Peter Hirsch*

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

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## **B. Non-Metallic Materials**

### **I - CERAMICS AND COMPOSITES**

#### ***Nanocomposite ceramics for technical applications***

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

The project is aimed at use of alumina - silicon carbide ceramic nanocomposites in applications where wear and abrasion resistance are important. The project is focussed on the surface mechanical properties of sintered ceramic nanocomposites. There are two main aims - (a) to understand the mechanisms of their improved properties over normal alumina ceramics; (b) to produce materials usable in real industrial applications. This project is in collaboration with Morgan Matroc.

#### ***Composites based on synthetic opal***

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

Novel composites have been prepared by filling the regular voids in synthetic opal by guest materials such as tellurium, InSb, GaAs, etc.. The opal is a cubic-close-packed lattice of SiO<sub>2</sub> spheres, and it has been found that the guest materials may be present as a single-crystalline, 3-D networks, giving unusual properties. (\*In collaboration with the Ioffe Physical-Technical Institute, St Petersburg, Russia, supported by the Royal Society)

#### ***Structure and properties of 'Hardide' coatings***

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

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

#### ***High temperature strengthening of zirconia ceramics***

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

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

#### ***Self-bonding nanocomposites***

*D. Colvin, Dr. A.M. Cock, Dr. S.G. Roberts*

Some preliminary experiments show that alumina-silicon carbide "nanocomposite" ceramic components can be joined together simply by heating them to about 1200C; this has potential applications in the manufacture of complex components. The project investigates the joining mechanism, which we believe to be due to oxidation of the SiC nanoparticles, and studies how additives can enhance "joinability" (especially by reducing the temperature needed) and the strength of the joints.

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

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

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

#### ***Residual stresses and mechanical properties in oxide matrix nanocomposites***

*N. Wain, Dr. R.I. Todd*

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

***Crack bridging forces in chromium carbide/alumina platelet composites***

*T. Joseph, Dr. R.I. Todd*

Previous work in this department has shown that composites in the alumina/chromium carbide system have unusual interfacial properties which promote toughening by crack interface bridging. This project aims to build on this work by fabricating chromium carbide/alumina platelet composites and investigating their fracture properties at macroscopic and microscopic levels, with the aim of producing a discontinuously reinforced material with properties approaching those of long fibre composites. The stresses in individual platelets as they dissipate energy during pullout are being measured using optical fluorescence microscopy, and the results used to model crack propagation in these materials.

***Perovskite-based ceramic nanocomposites***

*H. Wang, Dr. R.I. Todd*

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

**II - BIOMEDICAL MATERIALS**

***Crystallographic texture determination of calcium phosphates***

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

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

***Bone biomaterials bonding***

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

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

***In situ formation and electrodeposition of active coatings***

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

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

***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)

***Mechanical properties of biocomposites***

*D. Gotor, Dr. J.T. Czernuszka*

Composites based on natural systems are being made and their dynamic mechanical and fracture response determined. New models of how this class of materials deform are being formulated.

***Macro-assembled spheres of apatite***

*O. King, 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, EPSRC)

### ***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\*, Dr. D.G. Bucknall*

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

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

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

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

### ***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 ferroelectric, elastic and optical properties.

### ***An improved bone-implant interface***

*A. Walpole, M. Karlsson\*, Dr. E. Palsgard\*, Dr. L. di Silvio\*\*, Professor V. Baranauskas, Dr. P.R. Wilshaw*

A new coating for metal implant prostheses is being developed. This entails bonding a layer of porous alumina to the metal surface and filling the pores with a bioactive material such as bioactive glass. It is hoped that in this way the strength of the interface between the bone and implant will be improved whilst the mechanical properties of the implant are maintained. (\*Centre for surface biotechnology, Uppsala University, Sweden; \*\*UCL, UK)

### ***Three Dimensional Scaffolds for Tissue Engineering***

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

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

## **III - POLYMERS**

### ***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)

### ***Oxidative degradation of polymers***

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

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



### **Diffusion in composite materials**

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

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

### **Effects of molecular architecture on polymer interdiffusion**

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

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

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

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

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

### **Surface crystallisation of polymers**

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

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

### **Diffusion and solubility in polymers**

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

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

### **Real time studies of polymer interfaces**

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

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

### **Gloss of polymers**

*Dr. H.E. Assender*

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

### **Ion beam lithography**

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

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

### **Luminescent Conjugated Polyrotaxanes**

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

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

### **Mechanisms of Glass Transition of Polymer Thin Films**

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

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

### **Unstable polymer-polymer interfaces**

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

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

### **Long range ordering of block copolymer**

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

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

### **Structure and properties of silk**

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

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

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

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

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

### ***Electric Field Induced Orientation of Zwitterionic Telechelic Polymers***

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

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

### ***Network formation in epoxy/amine resins***

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

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

### ***Vacuum Web processing***

*Dr. H.E. Assender*

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

### ***Coating polymer films***

*D. Howells, Dr. H.E. Assender, Dr. C. Borman\**

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

### ***Influence of heterogeneous surfaces on polymer thin film behaviour***

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

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

### ***Nano-structures derived from polyrotaxanes***

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

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

### ***Microstructure of polymeric materials***

*Dr. D. Vesely*

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

### ***Patterning of Polymer Thin Films***

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

Thin polymer films can demonstrate interesting dewetting behaviour on non-wetting surfaces. By capping such unstable thin films by thick rigid layers this dewetting can be prevented. By selectively capping these inherently unstable thin films by semi-rigid capping layers it is possible to produce a surface topology with a random wave morphology. This

project aims to understand this phenomena and ways to control the feature size and more particularly anisotropy of the resulting structures.

### ***Microfluidic phase mixing and demixing***

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

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

### ***Polymer-Plasticiser Diffusion***

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

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

### ***Behaviour of model ionomer solutions***

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

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

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

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

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

## **IV - PHOTOVOLTAIC MATERIALS**

### ***The optoelectronics of organic photovoltaic materials.***

*Dr. M.J. Carey, Dr. H.E. Assender, Dr. P.L. Burn\*, Dr. Y. Tsukahara\*\**

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

### ***Device manufacture and characterisation of organic photovoltaic materials***

*Dr. K.R. Kirov, Dr. H.E. Assender, Dr. Y. Tsukahara\**

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

***Synthesis of novel organic materials for photovoltaic devices***

*Dr. G.R. Webster\**, *Dr. H.E. Assender*, *Dr. P.L. Burn\**, *Dr. Y.Tsukahara\*\**

For the development of novel organic photovoltaic materials, various organic materials will be synthesised for the construction of nanoscale architectures or improved response to heat treatments for example. (\*Dyson Perrins Laboratory, Oxford University, \*\*Toppan Printing Company Ltd) (Supported by the Toppan Printing Company Ltd.)

***Deposition and characterisation of nanoporous conducting oxide films***

*Z. Xie*, *Dr. B.M. Henry*, *Dr. C.R.M. Grovenor*, *Dr. Y. Tsukahara\**

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

***Modelling of polymer-conducting oxide photovoltaic devices***

*Dr. V. Burlakov*, *Professor A.P. Sutton*, *Dr. Y. Tsukahara\**

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

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## ***C. Electronic Materials and Devices***

### **I - SUPERCONDUCTING MATERIALS**

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

#### ***Microstructural characterisation of superconducting materials***

*Dr. H. Wu, S. Speller, C.J. Dark, S. Latif, C.J. Salter, Dr. C.R.M. Grovenor*

Superconducting ceramic samples fabricated in bulk, wire and thin film form are being characterised by X-ray diffraction and electron microscopic techniques. Of particular interest is the determination of the phase distribution and alignment, grain boundary structure and chemistry, and impurity phase chemistry in materials prepared both within the University and by a number of collaborators, and the correlation of these features with critical current measurements. High resolution and analytical TEM, XRD texture analysis, electron microprobe proton microprobe and orientation imaging microscopy techniques are being used to study the key microstructural features - especially the grain boundary structure and properties. (Funded by EPSRC and in collaboration with Oxford Instruments, University College London, Cambridge University)

#### ***Development of novel metallic substrates for superconducting tapes***

*R.M. Whiteley, Dr. J. Moore\*, Dr. C.R.M. Grovenor, Dr. J.M. Sykes*

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

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

*R.M. Whiteley, Dr. J. Moore\*, Dr. C.R.M. Grovenor, Dr. J.M. Sykes*

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

#### ***Synthesis and microstructure of MgB<sub>2</sub> precursor powders and wires***

*L. Goodsir, Dr. H. Wu, N. Allsop, C.J. Salter, Professor P.J. Dobson\*, Dr. C.R.M. Grovenor, Dr. P. Kovac\*\**

MgB<sub>2</sub> is a most promising new superconducting material for high current applications at temperatures below 30K. We are studying new methods for the chemical synthesis of high quality MgB<sub>2</sub> powder with controlled particle size and impurity content. At the same time we are collaborating with the Kovac research group in Slovakia on the analysis of the microstructure of high current wires fabricated with commercial starting powder. XRD, SEM and EPMA analysis are all key aspects of the work. (\*Academic Director of the Oxford University Begbroke Business and Science Park, \*\*Institute of Electrical Engineering, Slovak Academy of Sciences)

### ***Fabrication of thin films of superconducting ceramics***

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

Sputtering and post annealing processes are being used to deposit thin films up to 3" in diameter of Tl-based superconducting ceramics and buffer layers. The mechanisms of growth and the composition and microstructure of the films are being investigated as a function of deposition parameters, and related to the superconducting and microwave properties. Vicinal substrates are also being used to achieve off axis growth for specific device designs. The aim is produce optimised high Jc/low Rs materials for a wide range of practical applications.

(Funded by EPSRC and in collaboration with Department of Physics, University College London, Department of Engineering Science\*, Oxford, Department of Metallurgy and IRC in Superconductivity, University of Cambridge, Department of Physics, Department of Electrical Engineering, University of Birmingham)

### ***Microwave device fabrication from superconducting thin films***

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

Prototype passive microwave components (filters, resonators, mixers and correlators) are being fabricated in 2 inch diameter TlBaCaCuO thin films on LaAlO<sub>3</sub> and MgO substrates, and their performance compared with superconducting properties to optimise preparation processes. World-class surface resistance values are routinely achieved, and a range of novel device types are being studied particularly for applications in digital TV systems. More fundamental properties of thin films containing an array of defects are also being investigated. (Funded by EPSRC and in collaboration with Department of Physics, University College London, Department of Engineering Science\*, Oxford, Department of Metallurgy and IRC in Superconductivity, University of Cambridge, Department of Physics, Department of Electrical Engineering, University of Birmingham)

## **II - MAGNETIC MATERIALS**

### ***Composite magnetic nanoparticle systems***

*A. Eggeman, W. Nicholson, Professor A.K. Petford-Long, Professor P.J. Dobson\**

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

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

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

The MBE system in the Clarendon Laboratory is being used to grow epitaxial spin-valve structures and exchange-bias films, so that the exchange-biasing mechanism (vital to the operation of modern hard-disk read-heads) can be studied in the absence of features such as grain boundaries. The magnetisation reversal of the films is being characterised using Lorentz electron microscopy and their microstructure is being analysed using HREM and composition mapping. (\*Clarendon Laboratory, Oxford) (Funded by EPSRC)

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

*Professor A.K. Petford-Long, Dr. H. Laidler\*, Dr. M. Kief\*\*, Professor K. O'Grady\**

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

### ***Studies of patterned magnetic thin films***

*N.W. Owen, T. Bromwich, Dr. R. Langford, Professor A.K. Petford-Long*

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

### ***Spin-tunnel junctions based on magnetic layered films***

*Professor A.K. Petford-Long, J. Imrie, Dr. B. Warot, Dr. T.C. Anthony\*, Dr. J.A. Brug\**

Spin-tunnel junction devices are magnetic layered systems which exhibit giant magnetoresistance. The aim is to develop these systems for applications as magnetic field sensors and/or magnetoresistive memory elements. (\*Hewlett-Packard Labs.) (Funded by Hewlett-Packard Labs. and EPSRC via a collaboration with the Univ. of Cambridge and Univ. of Plymouth)

## **III - SEMICONDUCTOR MATERIALS**

### ***Quantum wires and dots***

*Dr. J.L. Hutchison, F. Ito, N. Allsop, Professor P.J. Dobson\*, R.N. Taylor, Dr. O.V. Salata, Dr. G. Wakefield\*\**

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

### ***Improved Si substrates for microwave applications***

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

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

### ***Polysilicon emitter bipolar transistors***

*Dr. C.D. Marsh, Dr. G.R. Booker, Professor P. Ashburn\*, Professor D.J. Roulston\*\**

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

### ***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 strain distributions in semiconductors***

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

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

### ***Room temperature light emission from silicon***

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

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



***Impurities and dislocations in Si wafers***

*Dr. S. Senkader, A. Giannattasio, Dr. R. Falster\*, Dr. P.R. Wilshaw*

The interaction between impurities such as O, N and H and defects such as dislocations and precipitates is being studied. In particular the diffusivity and effect of H on diffusivity in the range 350-700°C is being investigated together with the locking of dislocations by impurities and the mechanism by which precipitates weaken wafers. One of the aims of the project is to understand impurity-defect interactions so that stronger Si wafers may be manufactured. (\*MEMC, Italy) (Funded by MEMC)

***Semiconductor quantum dots***

*Dr. P. Moeck\*, Professor N.D. Browning\*, Dr. G.R. Booker*

Structural studies are being performed on Group 3-5 and Group 2-6 semiconductor quantum dots using Z-contrast STEM and HRTEM lattice imaging. Crystal lattices and atomic ordering within individual quantum dots are being determined and related to optical and electrical properties. (\*Physics Department, Illinois University, Chicago)

***Quantum dots***

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

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

**IV - DISPLAY MATERIALS**

***Non-lithographic definition of sub-micron field emitter structures***

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

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

***Development of electroluminescent display based on phosphorescent materials***

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

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

***Dendrimers as multifunctional materials for OLEDs***

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

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

***Carbon nanotube field emission displays***

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

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

### ***OLED interface engineering using ultra-thin inorganic layers***

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

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

### ***Material issues in degradation of OLEDs***

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

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

## **V – QUANTUM INFORMATION PROCESSING**

### ***Nanoelectronics at the Quantum Edge***

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

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

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

### ***ESR Study of Carbon Nanostructures for Quantum Computing***

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

Molecules of N@C60 have an exceptionally sharp ESR signal corresponding to long-lived electronic spin states. The suitability of these states for storing quantum information is being evaluated. A chain of interacting spin-active molecules may be realised by filling a carbon nanotube. The possibility of using such a chain for processing quantum information is being considered. See [www.nanotech.org](http://www.nanotech.org) (\*Department of Physics)

### ***Bio-molecular Quantum Computation***

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

This study aims at implementing the use of the resonant transfer of excitons in complex bio-molecular systems (e.g., the purple bacteria *Rhodospirillum rubrum*) for quantum computing purposes. We have performed some calculations that support the feasibility of such an approach, but this study is still in progress and needs further exploration. (\*Clarendon Laboratory, Department of Physics) (This work is supported by EPSRC as part of the Foresight LINK Award Nanoelectronics at the Quantum Edge.)

**Assembly of Molecular Arrays in Single-Walled Carbon Nanotubes**

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

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

**STM/STS of nanotubes**

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

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

**A Quantum Field Theoretical Approach to Decoherence of Quantum Dot Registers**

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

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

**Theory of Quantum Computing with Excitons in Quantum Dots**

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

The strength and nature of the interactions between excitons in self assembled quantum dot structures will determine how suitable they are as quantum information processors. We have been performing theoretical investigations into these interactions and have recently shown how to optimize such a molecule so that simple quantum logic can be performed. We have proposed two alternative possibilities: one which uses coupling to a light field to control the quantum state of the molecule, and another which uses the internal interactions to do this. See <http://www.nanotech.org/research/theory/QDrelated> for more details.

**Physical embodiment of qubits**

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

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

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## **D. Processing**

### ***Mechanical properties and microstructural evolution of semi-solid alloys***

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

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

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

*M.K. Hedges, Dr. I.C. Stone, Dr. P.S. Grant*

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

### ***Reliable compact capacitors for aerospace applications***

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

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

### ***Novel manufacturing routes for Al products***

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

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

### ***Rapid spray formed tooling***

*T. Rayment, P. Jones\*, Dr. V. Tsachouridis\*, Dr. Z. Djuric, Dr. S. Hoile, Dr. S. Duncan\*, Dr. P.S. Grant*

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

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

*Dr. S. Hogg, Dr. I.G. Palmer, Dr. P.S. Grant*

A state-of-the-art 80kg Al spray forming plant has been installed and commissioned in a dedicated laboratory. Research focuses on production and evaluation of low density Al-Mg-Li and 7XXX alloys by spraycasting; characterisation of microstructure; investigation of secondary processing on the development of the microstructure and the resulting mechanical properties; definition of new compositions and processing conditions for optimised alloys; and scale-up to billet sizes suitable for forging and component trials. (Funded by EPSRC and Joint Infrastructure Fund and in collaboration with Southampton University, Imperial College, BAE Systems and QinetiQ).

### ***Sedimentation studies in Al alloys***

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

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

**Direct chill casting of Al alloys***Dr. K.A.Q. O'Reilly*

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

**Spray formed silicon-aluminium alloys for electronic packaging applications***A. Lambourne, Dr. P.S. Grant*

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

**Modelling, microstructure and properties of nickel superalloys processed by centrifugal spray deposition***Dr. P.S. Grant, Dr. A. Dowson\*, Dr. M. Jacobs\**

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

**Control of temperature during vacuum plasma spraying***Dr. P.S. Grant, E. Davies\*, Dr. S. Duncan\**

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

**DC and shape casting of wrought Al alloys***I. Davidson, Dr. K.A.Q. O'Reilly, Dr. I.C. Stone, Dr. M.R. Jarrett\**

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

**Melt conditioning of Al alloys***M. Lovis, Dr. K.A.Q. O'Reilly, Dr. I.C. Stone, P.G. Enright\**

This project is developing novel thermal and chemical melt conditioning procedures for the control of microstructures during casting, providing evaluation and measurement technologies for the same, and will demonstrate the benefits of melt conditioning on (i) the manufacture of thin walled, high integrity automotive sand and die castings; and (ii) the selection of preferred intermetallic phases during DC casting. (\* N-Tec Limited)

**Squeeze casting and semi-solid processing of Al alloys***C.D.J. Manson-Whitton, Dr. I.C. Stone, Dr. K.A.Q. O'Reilly, Professor B. Cantor\**

An UBE 350 tonne squeeze casting and semi-solid processing machine is has been installed in the department and will be used to investigate the effects of alloy composition, and processing parameters on the microstructures and properties of squeeze cast and semi-solid processed Al alloys. (Funded by JREI and Luxfer Group)(\*University of York)

**Manufacture and characterisation of nanostructured aluminium alloys**

*Dr. M. Tomut, Dr. D. Crespo, N. Grennan-Heaven  
Dr. I.C. Stone, Professor B. Cantor\**

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

**Carbon fibre reinforced magnesium**

*M. Russell-Stevens, Dr. K.A.Q. O'Reilly, Dr. R.I. Todd, P. Schultz\**

Microstructural investigation of long fibre carbon fibre reinforced magnesium alloys manufactured by squeeze casting, as a function of casting parameters. (\*Leichtmetall Kompetenzzentrum Ranshofen) (Funded by EPSRC)

**Manufacture and characterisation of nano-quasicrystalline aluminium alloys**

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

Al-base nanocomposite materials containing high volume fractions of quasicrystalline dispersoids are being produced by rapid solidification techniques. Particular emphasis is being placed on the dependence of alloy composition on the ability to form the quasicrystalline phase during quenching. (\*University of Buenos Aires; \*\*University of York) (Funded by EU and British Embassy Korea S&T Fund)

**Multicomponent alloys**

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

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

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## ***E. Phase Transformations, Surfaces and Interfaces***

### **I - PHASE TRANSFORMATIONS**

#### ***Structure and crystallisation kinetics of optical and magnetic nanocomposites***

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

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

#### ***Cyclic phase transformations***

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

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

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

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

Crystals of various salts and metals grown within single-wall carbon nanotubes are effectively 1-D wires, with a range of interesting physical properties which arise from their unique configurations, We are exploring ways of growing these structures, which are characterised by HREM, EDX and EELS. Their physical properties are also under investigation. (\*Inorganic Chemistry Laboratory)

#### ***The development of a high temperature single pan scanning calorimeter.***

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

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

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

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

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

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

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

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

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

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

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

1. How do precipitate nucleation and growth, structure and composition depend on irradiation and thermal conditions?
2. What are the mechanisms of copper transport?

3. What is the effect of bcc-9R transformation on the copper-precipitate binding energy and overall kinetics?
4. What is the hardening mechanism of the coherent bcc precipitates?
5. Do dislocations cut through bcc precipitates, leaving them essentially unchanged, or do they induce transformation to the 9R structure?
6. What is the hardening mechanism of the incoherent 9R precipitates?
7. How are the mechanisms influenced by incorporation of other alloying elements?

## II - OXIDATION AND CORROSION

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

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

The variation with depth of the composition of corrosion layers on buried metal objects can provide the archaeologist with valuable information relating to the burial conditions of the object. In some cases these layers can be very thick (up to 1mm) and so normally, destructive methods such as sectioning are used to characterise the layers. The technique developed here uses a micro-focused high power pulsed Nd:YAG laser to ablate the corrosion layer in a series of controlled steps, while monitoring the composition of the exposed surface using PIXE and RBS in the external beam facility of the Oxford Scanning Proton Microprobe. The region of the surface removed by the laser beam is typically less than 500µm diameter and so, by comparison with other sampling techniques, the effect on the appearance of an object is minimal. (\*University of Surrey)

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

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

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

### ***Corrosion protection of metal packaging by organic coatings***

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

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

### ***Ageing of organically coated metal surfaces***

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

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

### ***The origin of corrosion in coated metal packaging containers***

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

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



### III - SURFACE REACTIONS AND CATALYSIS

#### ***Controlled atmosphere analytical electron microscopy***

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

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

#### ***In-situ observation of solid-state reactions***

*Dr. J.L. Hutchison, Dr. M.J. Sayagues de Vega\**

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

#### ***Catalytic atom probe***

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

A specially adapted atom probe, incorporating a gas reaction cell, is being developed in order to permit the atomic scale study of catalytic reaction processes. (Funded by EPSRC and in collaboration with Johnson Matthey and Omicron Surface Science Ltd.)

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## F. Characterisation

### I - SCANNING TUNNELLING AND ATOMIC FORCE MICROSCOPY

#### **Direct measurement of interatomic potentials**

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

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

#### **Atomic resolution AFM**

*L. Giberti*, *Professor J.B. Pethica\**

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

#### **New force microscopy techniques in ambient**

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

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

#### **Forces on single atoms in STM**

*Professor J.B. Pethica\**, *L. Giberti*, *Dr. J. Nieminen\*\**

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

#### **Room temperature manipulation of surface atoms**

*Professor J.B. Pethica\**, *Dr. R.G. Egdell\*\**

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

#### **STM & AFM of metals on oxides at variable temperature**

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

A new variable temperature STM and XPS system is used to study catalytic oxides and metal islands thereon. Surfaces under investigation include SnO<sub>2</sub>, WOn and tungsten bronzes, ZnO. (\*Trinity College, Dublin; \*\*Inorganic Chemistry Laboratory; \*\*\*Physical Chemistry Laboratory) (Funded by EPSRC)

#### **Growth and characterization of quantum silicide and nitride islands**

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

The growth and properties of silicide and nitride islands are studied, with a view to discovering materials systems that may be useful for quantum structures. Islands are grown in our variable temperature STM, and examined in situ. We study both metallic and semiconducting islands. We investigate factors that affect their shape and size distributions, the phases that are present, and the surface structures and electronic properties. Atomistic and multiscale modelling enables the structure of surfaces and interfaces to be elucidated, and the distribution of island types and sizes to be accounted for.

***Nanostructures on the SrTiO<sub>3</sub> (001)******Surface***

Dr. M.R. Castell

Atomically resolved scanning tunnelling microscopy of the SrTiO<sub>3</sub> (001) surface reveals that certain treatments give rise to two types of self assembled nanostructures. The one dimensional structure type consists of perfectly straight lines that run in <100> directions and have a minimum separation of 2.4 nm. The other structures are dots that on closest packing form 2.4 nm x 1.6 nm arrays. It is proposed that both structure types are formed through nano-crystalline growth of non perovskite phases on the surface. Further characterization and metal island growth on these surfaces is currently being carried out. (Funded by The Royal Society)

***AFM of aqueous bio-systems***

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

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

***Atomic structure of oxide surfaces***

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

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

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

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

The growth of self-assembled quantum nitride nanostructures (InGaN, AlGaIn) by molecular beam epitaxy (MBE) is studied in-situ by elevated-temperature scanning tunnelling microscopy (STM) and electron diffraction to investigate nucleation and elucidate growth modes. The size and shape distributions of quantum dots are studied to develop a nanostructure diagram as a function of composition and growth parameters. (\*TU-Ilmenau, Germany) (In collaboration with Hewlett-Packard Laboratories.)

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

***Atom probe microanalysis techniques***

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

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

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

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

Thin metallic layered films with applications in information storage are being grown by sputter deposition and atom probe tips are being fabricated from these layers by FIB milling. The layer composition and interface nature are being studied using both three-dimensional atom probe analysis, in parallel with HREM studies of the crystal structure of the films. Experimental analysis of interface changes with thermal annealing is being compared with simulations of the interdiffusion process. (\*Seagate Technology) (Funded by EPSRC and Seagate Technology)

**Early stages of precipitation in 6XXX automotive sheet**

*D. Vaumousse, Professor A. Cerezo*

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

**Atom probe studies of 2xxx Al alloys**

*L. Davin, Professor A. Cerezo*

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

**Early stages of precipitation in 7xxx series aluminium alloys**

*Dr. G. Sha, Professor A. Cerezo, Dr. A. Alam\**

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

**3D Reconstruction of atom probe data**

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

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

**Thermal ageing of steels**

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

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

**Scanning atom probe**

*T.J. Godfrey, Professor A. Cerezo, Professor G.D.W. Smith*

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

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

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

**High resolution electron microscopy (HREM)**

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

***Analytical electron microscopy (AEM)***

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

***High resolution analytical electron microscopy***

A JEOL 2010 high resolution electron microscope has been installed in 1994. This instrument combines high spatial resolution (down to 0.19 nm) with a two nanometre diameter electron probe for nano-diffraction or convergent beam diffraction. An energy-dispersive X-ray analysis capability and an on-line TV imaging system make this a very versatile instrument. It is being used in a wide range of projects, with particular emphasis on microstructural characterization of nanocomposites.

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

Early in 1999 the Department installed and commissioned the UK's first 300 kilovolt field-emission-gun high resolution electron microscope. This instrument, a JEOL 3000F, is fully equipped with a comprehensive range of advanced analytical facilities, including light-element sensitivity EDX, parallel electron energy loss spectroscopy (PEELS), energy-filtered imaging (GIF), an electrostatic biprism for electron holography, a high performance CCD camera and a piezoelectric, drift correcting specimen stage. With a capability of microanalysis and electron diffraction from areas down to  $<0.4\text{nm}$  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 ( $<1 \times 10^{-10}\text{mbar}$ ). The instrument is used primarily for combined structural and chemical analyses of interfaces.

***Scanning electron microscopy (SEM)***

The JEOL JSM-840F field emission scanning electron microscope (FEG-SEM) was installed for the purpose of obtaining images of crystal defects in bulk materials using the electron channelling contrast imaging (ECCI) technique developed in the department. This machine can produce both images of single dislocations and electron channelling patterns (ECP) and is being used to investigate sub-surface dislocation arrays and networks in partially relaxed epilayer materials and also to study defect distributions around crack tips. A JEOL JSM-6300 scanning electron microscope has also been installed for electron diffraction experiments. This has a LaB<sub>6</sub> 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.

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

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

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

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

As part of a major research grant, the Department has secured funding which enables us to work closely with an electron microscope manufacturer in developing the next generation of high performance electron microscopes. The new instrument 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.

### ***The structure of copper precipitates in age-hardening steels***

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

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

### ***Polyhedral and cylindrical metal chalcogenides***

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

Closed polyhedral structures of the layered materials WS<sub>2</sub>, MoS<sub>2</sub> and other chalcogenides have recently been discovered. They are in the form of concentric, polyhedral shells, somewhat similar to the "buckyball" and "fullerene" carbon cage compounds. Their formation and structures are being investigated by high resolution electron microscopy. Their possible use as high-performance solid lubricants is being investigated. (\*Weizmann Institute, Israel) (Funded by UK-Israel Research Fund)

### ***Electron back scatter diffraction***

*Dr. A.J. Wilkinson*

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

### ***NanoSIMS analysis of metallic and electronic materials***

*C. Dark, S. Ahmed, Dr. G. Taylor, Dr. C.R.M. Grovenor, Professor J.M. Titchmarsh, Professor J. Foord\**

A Cameca NanoSIMS50 has just been installed at the Begbroke Business and Science Park. This equipment is a state-of-the-art machine for chemical analysis with high spatial resolution and very high sensitivity for most elements. We will use this new facility in projects where the accurate analysis of the distribution of dilute element is critical to developing a better understanding of the materials properties. Initial projects include;

- [1] Grain boundary doping studies in high temperature superconductors (with University of Augsburg)
- [2] Analysis of the distribution of H dopant in diamond films (\* Professor John Foord, Department of Chemistry,)
- [3] Light, interstitial element analysis in TiAl intermetallics
- [4] The chemistry of crack tips in structural alloys

### ***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)

### ***NanoSIMS analysis of Biological Materials***

*K. Smart, Dr. C.R.M. Grovenor, Professor J. Dilworth\*, Professor J.A.C. Smith\**

A Cameca NanoSIMS50 has just been installed at the Begbroke Business and Science Park. This equipment is a state-of-the-art machine for chemical analysis with high spatial resolution and very high sensitivity for most elements. 50% of the time on this new facility will be dedicated to studies of biological materials. The first two projects will be [1] the analysis of the mechanisms for heavy metal transport and accumulation in hyperaccumulator plants [2] the localisation of Rh complexes in a study of new imaging and therapeutic agents for hypoxic tissue. (\* Professor Jon Dilworth Department of Chemistry, Professor Andrew Smith Department of Plant Sciences)

### ***Electron probe microanalysis of multicomponent materials***

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

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

### ***Development of transmission electron microscopy for studies of crack tips***

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

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

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

*Professor J.M. Titchmarsh*

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

### ***Structure of amorphous materials***

*Professor D.J.H. Cockayne, Dr. D. Ozkaya, Dr. M. Doeblinger, Dr. D. Nguyen Manh,*

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

### ***In-situ TEM studies of magnetic domain structure***

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

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

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

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

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

### ***Development of an advanced FIB system for micromachining applications***

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

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

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

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

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

### ***Preparation of TEM specimens for high resolution electron microscopy***

*Dr. R.M. Langford, S. Lozano-Perez, Professor A.K. Petford-Long*

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

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

*Dr. R.M. Langford, Dr. Y.Q. Ma, Professor A.K. Petford-Long, Professor A. Cerezo, Dr. P. Clifton\*, Dr. D.J. Larson\**

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

### ***Quantum dot and quantum well structures***

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

The geometry and composition of quantum dots in semiconductor materials is being investigated with a range of electron optical techniques including HREM, energy filtered EM, and image simulations. (\*University of Sydney; \*\*Department of Physics)

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

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

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

### ***Electron Energy Loss studies of nanostructures***

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

The electron energy loss fine structure of nanostructures is being investigated both theoretically and experimentally, using high resolution energy loss techniques.



**Remote Microscopy**

*Professor D. Cockayne, Professor P. Jeffreys\*, Professor G.D.W. Smith, Professor J. Titchmarsh, Dr. P.J. Warren, Professor A. Cerezo*

Remote access to electron microscopes is being developed. The aim is to develop a capability of persistent and pervasive access, using the e-Grid.

**Nanometer scale induced structure between amorphous layers and crystalline materials**

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

Interfaces between amorphous/glassy layers and crystalline materials are playing an increasingly important role in the properties of manufactured ceramics and composites, especially as they move towards the nanometre scale. The goal of this project is to achieve a complete computational and experimental description of the structure and basic properties of crystal/glass interfaces, for the purpose of improving materials properties. This project is a joint project funded by EU and NSF between participants at \*Max Plank Institute, Stuttgart, \*\*University of Karlsruhe, \*\*\*CEA, Saclay, +MIT, ++University of Pennsylvania, +++Rutgers University, †University of Missouri-Kansas; and ††Lawrence Berkeley Lab, San Francisco. (††† now at Dept Engineering Materials, University of Sheffield)

**Analysis of oxide layers on nitrocarburised steels**

*T. Vaughan, Professor J.M. Titchmarsh, Dr. M.L. Jenkins*

Nitrotec is a company based in Birmingham that owns a patent on gaseous nitrocarburising. This process develops iron nitride layers ranging from 5 to 50 microns thick on top of a nitrogen rich zone in the substrate. This layer may be further developed with a post oxidation that leaves an oxide layer on top of the compound layer, which is between 0.5 to 5 microns thick. This treatment has benefits particularly for corrosion and wear resistance. In this project we shall carry out an analysis of the compound and oxide layers in order to better understand their structure and morphology, which at present are not well known. Of particular interest is the interface between the compound and oxide layers.

**TEM investigation of stress corrosion cracking in Inconel 600**

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

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

## IV - RADIATION DAMAGE

**Mechanisms of embrittlement in reactor pressure vessel steels**

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

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

**The influence of nanometer-scale defects on anomalous absorption in the TEM**

*Dr. M.L. Jenkins, Professor J.M. Titchmarsh, L. Scruby, Dr. C.J.D. Hetherington*

Single point defects and very small point-defect clusters are expected to enhance anomalous absorption by scattering electrons out of the objective aperture in diffraction-contrast images. This is being investigated experimentally by measurements of the decay of thickness fringes with foil thickness in foils containing high densities of very small defects. The aim is to determine whether such measurements can provide information on populations of defects too small to be imaged in the TEM using any of the available imaging techniques.

**Contributions of Inelastically Scattered Electrons to Defect Images.**

*Dr. M.L Jenkins, Dr. C.J.D. Hetherington, Dr. M.A. Kirk\*, Dr. R. Twiston\*\**

The availability within the department of the JEOL 3000F FEGTEM equipped with a Gatan Imaging Filter (GIF) and CCD camera has opened up new opportunities for exploring more systematically the advantages of energy-filtered imaging and diffraction, and determining more precisely the contributions to images and diffraction patterns of inelastically scattered electrons. A particularly promising new technique involves measurements of Huang scattering near weakly excited diffraction peaks from isolated small point-defect clusters. The asymmetry in the Huang scattering immediately reveals the interstitial or vacancy nature of the cluster. This technique is now being explored systematically. (\*Argonne National Lab; \*\*University of Illinois)

**Quantum Electron Microscope Imaging of Nanoclusters under Weak-Beam Conditions**

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

This project is focused on the development of a new approach to the interpretation of electron microscope images of nanoclusters. The approach is based on the theory developed by Howie and Basinski, where quantum interference between non-parallel diffracted electron beams is taken into account. Our work involves further development of a computer code implementing the original Howie and Basinski equations written at the University of Minnesota by the group led by Professor C B Carter, to allow image simulations under weak-beam diffraction conditions of nanoclusters of complex morphology. These image simulations will be matched with experimental images of small clusters produced by interaction of high-energy particles with metallic crystalline films. (\*EURATOM/UKAEA Fusion Association; \*\*University of Minnesota; \*\*\*Argonne National Laboratory)

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## **G. Modelling and Simulation**

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

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

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

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

### **Studies of amorphous carbon films by electron diffraction and modelling**

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

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

### **MBE growth of spintronic materials**

*Professor D.G. Pettifor, Dr. D. Nguyen Manh, Professor M.W. Finnis\*, Dr. X. Zhou\*\*, Professor H. Wadley\*\**

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

### **Power dissipation in metallic nanowires**

*Professor A.P. Sutton, Dr. T.N. Todorov\*, Dr. J. Hoekstra\**

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

### **Modelling phase change materials**

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

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

### **Modelling diffusional phase transformations in the presence of elastic interactions**

*Professor A.P. Sutton, Professor A. Cerezo, Dr. R.E. Rudd\*, D. Mason*

Earlier work has shown the necessity of using a vacancy mechanism of diffusion to model diffusional phase transformations in metallic alloys that occur on the 1-10 nanometre scale. Only when the correct mechanism of diffusion is used at the atomic scale will morphologies, kinetics and mechanisms of growth and coarsening be described correctly. In this work elastic interactions are being introduced to model transformations in alloys containing misfitting atoms. The elastic interactions are included by a new application of the Lanczos method. (Funded by EPSRC) (\*Lawrence Livermore National Laboratory)

### **Dynamical Ising model simulations of phase separation**

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

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

**Mapping of magnetisation distributions in thin layered films**

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

We have developed a method for quantitative mapping of the magnetisation in thin magnetic specimens at a high spatial resolution. The method is being used to study the magnetisation distribution in thin films and layered systems. (Funded by Hewlett-Packard Labs.)

**Modelling short fatigue crack growth through polycrystals**

Dr. A.J. Wilkinson

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

**Modelling adhesion between polymers and inorganic substrates**

Professor A.P. Sutton, Dr. S. Lorenz, Dr. T.R. Walsh\*

A new strategy for modelling adhesion between polymers and inorganic substrates has been developed. It is being applied to polymer adhesion issues of interest to the semiconductor industry. This project is part of an e-science collaboration called 'RealityGrid', funded by EPSRC.

**Fundamentals of brittle-ductile transitions**

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

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

**Carbon-based nanostructures**

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

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

**First principle studies of platinum aluminides**

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

The electronic structure, equation of state and phase stability of platinum aluminides 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 secondary electron emission from surfaces with inequivalent terminations**

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

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

**Modelling the structure of amorphous oxide films grown by vapour deposition**

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

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

**Modelling the evolution of cascades in fusion reactor materials**

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

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

**Unresolved issues in giant magnetoresistance**

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

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

**Modelling carbon nanostructures for quantum computing**

Professor D.G. Pettifor, Professor G.A.D. Briggs, Dr. D. Nguyen Manh, Dr. R. Scipioni

Tight binding and ab initio density functional codes are being used to predict the atomic and electronic structure of endohedral fullerenes inside single-wall carbon nanotubes, which are being investigated for their quantum computing potential. This is in close collaboration with in-house HREM, STM, EELS, Ramon and ESR experiments. (Funded by Foresight LINK Project, DTI and Hitachi Europe).

**Brittle-Ductile Transitions in Silicon**

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

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

**Current-induced effects in molecules**

Professor A.P. Sutton, M. Todorovic

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

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## ***H. Materials Science Based Archaeology***

The Materials Science Based Archaeology Group is concerned with the investigation of all aspects of the metallurgical process, from smelting to metal finishing, and from the first use of alloys in the 5th/4th millennia BC to the Industrial Revolution. The themes of the research can be broadly labelled as archaeological and metallurgical. In archaeology the research derives from post-excavation and museum-based projects involving the characterization of the products and residues of past metallurgical processes. The results are used to explore the place of metals in ancient economies and societies, how they were made, used, traded and re-cycled, how their properties were understood, and what processes were associated with their deposition and survival in the archaeological record. This work is supported by experiments designed to relate this material to the process variables which shaped its formation. These experiments also form a link with the metallurgical objectives of the group. These are to acquire a deep knowledge of the physical and mechanical metallurgy of the metals used in the past, so that we can see how they were understood in the past. The results can be surprising and demand novel research, for example to determine why some alloys have an exceptional ductility. This work also links directly with other areas of metallurgy by extending to  $6 \times 10^3$  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.

### ***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).

### ***Investigation of the relationship between slag inclusion compositions and welding practice***

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

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

### ***Effects of cremation on copper alloys***

*Dr. J.P. Northover*

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

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

*Dr. J.P. Northover, P. Nagy\*, P. Ramszl\*\*, 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)

### ***The characterisation of Islamic steels***

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

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

### ***Anglo-Saxon Ferrous Technology***

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

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

***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)

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

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

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

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

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

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

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

*Dr. J.P. Northover*

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

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

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

The requirements of museum collections have stimulated this project in non-destructive and minimally destructive analysis of ancient bronze. The aim is to use a laser to mill sub-millimetre diameter windows in the patina on selected bronzes and then use the SPM to analyse the metal as it is exposed, with the X-ray mapping facility employed to make basic metallographic observations. (\*University of Surrey)

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

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

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

***A study of Byzantine copper alloy metalwork***

*Dr. J.P. Northover, Dr. M. Saghih Beydoun\**

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

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

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

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

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