

# **Modelling of Materials and Processes**

**A review of activity and needs in the UK in  
response to the Technology Foresight exercise**

**H.R. Shercliff**

**Engineering Department  
Cambridge University**

**June 1997**

**Cambridge University  
Engineering Department  
Technical Report  
CUED/C-MATS/TR243**

# Synopsis

## Motivation for the Report

This report presents a review of materials modelling commissioned by the Institute of Materials (IoM) and Office of Science and Technology (OST), in view of the high profile given to materials modelling in the recommendations of the Technology Foresight exercise published in 1995.

The initial purpose of the report was to serve as a "position paper" for the IoM in its discussions of how to carry the Foresight objectives forward in this area. The overall aim is to promote the development of physically-based, industrially-useful models. Opinions have been sought by interviews and questionnaires, and from the published literature.

Given the importance of materials research, and modelling in particular, within current initiatives from EPSRC, DTI and other funding agencies, the report should be of interest to a wide community: government and other funding agencies, industrial and academic modellers, experimentalists who measure data intended either as input for models or for model validation, materials scientists and manufacturing process engineers, including managers responsible for modelling activities.

Materials modelling covers a vast range of activity - this is reflected in the responses to the questionnaire coming from fields as diverse as geological sciences, molecular modelling and high velocity impact, though the majority relate to work in the more traditional materials processing industries. The review has focused on "structural" materials - predominantly metals, polymers and composites. Within these classes of materials, consideration has not been given to extractive processing which falls within the remit of process and chemical engineering. "Functional" materials (semiconductors, superconductors, magnetic and optical materials, biomaterials etc) have also not been considered, nor have the less obvious "material processing" sectors such as food production. This selectivity is not intended to deny the importance of modelling in these areas, but is simply to keep the review manageable. Some opinions have been offered from these other areas of activity, and a number of the dominant issues will doubtless be familiar to those working in these areas. Separate studies would be required to highlight the more specific details which relate to the very different physical behaviour and industrial context of these areas.

This survey builds on an earlier study (Sargent, Shercliff and Wood, 1993) for the ACME Directorate of SERC, which considered almost exclusively metals manufacturing processes. The scope has been widened to non-metals, and consideration also given where possible to modelling of material performance in service. Expanding on the conclusions of the previous report, several key issues are raised concerning research priorities in materials modelling, the potential for greater academic-industrial collaboration, and training and educational needs in the UK.

Section 1 of the report summarises the relevant aspects of the Technology Foresight documents, and the response from the EPSRC. Section 2 discusses general issues and needs in materials modelling, while Section 3 provides more detailed comments on a number of key materials or process areas. Section 4 summarises with overall Conclusions and Recommendations.

## **Summary of Main Conclusions**

### **General industrial and academic perspectives**

- 1 The importance attached to materials modelling by Technology Foresight is fully endorsed by this survey of structural materials. Modelling also merits deeper consideration in extractive processing, building materials, functional materials, and food processing.
- 2 The industrial takeup of process modelling is very non-uniform across different materials processing sectors.
- 3 Most research activity and software is only accessible to large high-technology companies. A significant impact in SMEs requires more well-packaged PC-based software.
- 4 Centres of excellence in each industrial sector are needed to offer advice and training in modelling, to transfer expertise to industry (particularly SMEs), and for benchmarking software.
- 5 Modelling has a major role to play in Design for Manufacture by bringing processing into design at an appropriate level of complexity. Routine use of modelling can also benefit the overall efficiency of a manufacturing system.

- 6 Industrial modelling problems are no less demanding academically than purely scientific research. Defining research priorities in materials modelling requires input from both academics and industry, with scope for greater collaboration in every industrial sector.
- 7 Academic modelling too rarely leads to usable software for industry, but implementation in software should largely be the role of intermediate research organisations or spin-off companies.
- 8 Some academics comment that collaborative research and software output do not receive sufficient credit in Research Assessment Exercises, and that collaboration in modelling at the European level is also under-rated by funding agencies.
- 9 Multi-physics modelling and linking length scales are popular current themes. The benefits of adding greater complexity should be carefully argued for a given process or material problem.
- 10 Molecular calculations are making good headway in polymers. The best potential for atomistic methods in other materials appears to be for interfaces and surface behaviour, and for electronic materials.

### **Aspects of model building**

- 11 Computational power is not an issue except for certain complex 3D processing problems, or the most ambitious research process models. Increased computer power is absorbed far too readily in added complexity, rather than in more thorough use of an existing model.
- 12 Choosing the appropriate level of complexity is an essential element of all model building and use, and both analytical and numerical methods should be exploited.
- 13 FE methods are largely very mature, and further development would offer only modest benefit at present. Much more can be achieved by integrating microstructural and damage modelling with FE, in order to track the product state through multi-stage processing and service.
- 14 Software engineering developments are needed to enable smoother data transfer from design to production. Models are increasingly the basis for communication between suppliers and customers in industry.
- 15 The data needs of a modelling activity, both for input and to validate the output, should be considered (and costed) from the very start.

- 16 The new DTI MMP programme on measurement of materials parameters for processing rightly emphasises the importance of modelling. There is a need to make non-proprietary data for processing more widely available.
- 17 Interface properties, in particular friction and heat transfer, are critical in all materials process modelling. There is a need for research on micro-modelling of interfacial conditions, and the coupling of these models to macroscopic FE computations and to experiment.

### **Networking**

- 18 There is scope for more UK workshops covering a range of modelling activities, to promote collaboration. There is support for a well-organised directory of UK modelling activity, both on the Web and on a free CD.
- 19 Worldwide activity in materials modelling is very great - an international science-watch is very important in this field. The Web is not uniformly viewed as an efficient route to obtaining reliable information on modelling work.

### **Education and training**

- 20 Materials modelling is a key area to develop in degree courses at undergraduate and postgraduate level, combining materials science and engineering, numerical methods and software engineering.
- 21 The principal requirement in training modellers is establishing the right attitude, i.e. an open-minded approach, the ability to function in a team, and a clear view that a model is a tool to reach an end rather than an end in itself.
- 22 The EPSRC, and others running initiatives in training for universities and industry should consider whether greater emphasis can be given to materials modelling.

# Acknowledgements

This review of materials modelling has been greatly facilitated by the willingness of many academics and industrialists to offer both their time and opinions, either through meetings with the author, or by correspondence and completing a questionnaire. The topic is clearly attracting increasing interest in industry, with that awareness reaching the highest levels in management.

A partial list of those consulted during the review is given in the Appendix. I would particularly like to acknowledge the advice received in initiating the review from Prof. Mike Ashby and Prof. John Beynon; also the input of my co-authors on the earlier review for ACME, Dr. Phil Sargent and Bob Wood.

I wish to acknowledge the support of the review co-ordinators at the Institute of Materials, Mr. Robert McVickers and Dr. David Driver. The financial support of the Office of Science and Technology, co-ordinated by Mr. Brian Bradley and Mr. Brian Ferrar, is also acknowledged.

The assistance of Mr. Roger Burdett at EPSRC, and the Editorial staff of "Materials World", is acknowledged, for publicising the questionnaire used for the study. I am also grateful to Mr. Iain Cameron of EPSRC for making available the unpublished SERC report on processing, written by Dr. Graham Hollox.

This report is published by Cambridge University Engineering Department, as Technical Report CUED/C-MATS/TR243 (June 1997). The author wishes to thank Girton College, Cambridge, for assistance with publication costs.

Hugh Shercliff

Cambridge University Engineering Dept.  
Trumpington St., Cambridge, CB2 1PZ, UK  
tel/fax. (01223) 332627  
hrs@eng.cam.ac.uk

# Contents

---

<b>Synopsis</b>	i
<b>Motivation for the Report</b>	i
<b>Summary of Main Conclusions</b>	ii
General industrial and academic perspectives	ii
Aspects of model building	iii
Networking	iv
Education and training	iv

---

<b>Acknowledgements</b>	v
-------------------------	---

---

<b>Contents</b>	vi
-----------------	----

---

<b>Section 1:</b>	
<b>Materials Modelling and Technology Foresight</b>	1
<b>1.1 Introduction</b>	2
<b>1.2 Materials and Foresight: the rôle of modelling</b>	3
General observations from Technology Foresight	3
Sector highlights	3
The Materials Panel Report	6
Working Party on Aerospace Structural Materials	10
EPSRC response	10
Foresight Challenges in Materials	12
European dimension	12

---

<b>Section 2:</b>	
<b>Materials Modelling: General issues and needs</b>	13
<b>2.1 Introduction</b>	13
<b>2.2 Overview of issues in modelling materials during processing and in service</b>	14
Interpretation of "materials modelling"	14
Modelling processing and modelling performance	15
Appropriate modelling	16
Aspects of collaboration in materials modelling	17
A structured view of materials modelling	19

<b>2.3</b>	<b>Modelling: what is it for ?</b>	19
	Integration of processing into design, and product tracking	20
	Modelling of standard tests	21
	Modelling versus experiment	21
	Simple models and whole process models	22
	Sensitivity analysis and validation	23
<b>2.4</b>	<b>Modelling: identifying what is important</b>	24
	Choice of modelling method	24
	Boundary conditions	26
	Classification of modelling	26
<b>2.5</b>	<b>Data for Materials Modelling</b>	27
	Boundary condition data	28
	Models limited by data availability	29
	Initiatives in processing data measurement	29
<b>2.6</b>	<b>Scientific Developments in Materials Modelling</b>	30
	Modelling of material microstructure	30
	Linking length scales and multi-physics modelling	32
	Atomistics and molecular modelling	34
<b>2.7</b>	<b>Industrial take-up</b>	35
	Problems with technology transfer to industry	36
	Modelling entry costs	37
	Modelling centres	38
	Networking	39
<b>2.8</b>	<b>Education and training</b>	40
	Materials modelling in university courses	41
	Industrial perspective	43

---

## Section 3:

### Aspects of Materials Modelling in different material and process sectors

<b>3.1</b>	<b>Casting</b>	46
	Introduction	46
	Shaped casting modelling	46
	Modelling centres	49
	Other casting processes	50
	Data	51
	Underlying materials science	51
<b>3.2</b>	<b>Thermomechanical Processing of Metals</b>	53
	Introduction	53
	Modelling status	54
	Heat treatment	58

<b>3.3</b>	<b>Joining, Surface Engineering, Laser Processing, Ceramics and Powder Processing</b>	59
	Introduction	59
	Joining	59
	Surface engineering	61
	Laser processing	62
	Ceramics and powder processing	62
<b>3.4</b>	<b>Polymers and Composites</b>	64
	Modelling status: polymers	64
	Modelling status: composites	66
<hr/>		
<b>Section 4:</b>		
<b>Conclusions and Recommendations</b>		69
	Summary	69
	Critical aspects of modelling	70
	Industrial process modelling	70
	Academic modelling	72
	Technology transfer	73
	Computational aspects	73
	Data for modelling	74
	Education and training	75
	Carrying Foresight forward	75
<hr/>		
<b>Section 5:</b>		
<b>References</b>		77
<hr/>		
<b>Appendix</b>		79
	<b>List of people consulted</b>	79

# **Materials modelling and Technology Foresight**

## 1.1 Introduction

The Technology Foresight Programme aims to focus the UK's science, engineering and technology resources on improving national wealth and quality of life. Technology Foresight panels in 15 major sectors reported in 1995. The overall purpose and conclusions of the exercise have been well-documented elsewhere [e.g. OST, 1995a], and will not be covered again here.

The Materials Sector panel highlighted a number of high priority areas [OST, 1995b; Campbell and Humphreys, 1995]:

- models which relate materials composition, structure and process parameters to end product performance (with parallel improvements in supply of data, and methods of testing and evaluation)
- improved sensor materials and devices, and automated process control
- weight-saving technologies and higher temperature materials for specific applications
- processing technologies which improve the environment
- processing techniques for high temperature superconductors
- biomaterials which promote the restoration and repair of body tissue

Other areas which were considered to merit greater R & D investment were:

- rapid, low-cost, durable joining techniques
- surface engineering science and technology
- materials for mobile IT and telecommunications

Materials modelling was identified as an activity in its own right for linking composition to processing and microstructure, but it contributes to all of the other areas listed above, and can be central to these activities. It therefore emerges as a critical activity in implementing Foresight.

Amongst others, the Institute of Materials will play a major part in carrying forward the objectives of Foresight. The purpose of this report is to assemble information and opinions on materials modelling on behalf of the Institute, with the support of the Office of Science and Technology. By way of background for those not familiar with the Foresight reports, a brief overview is given of the possible roles of modelling. Principally these reflect the issues cited by the Materials Panel [OST, 1995b]. Materials of course also underpin many of the activities discussed by other Panels (for example, Chemicals, Defence and Aerospace, Food and Drink and so on). In the same way, modelling of materials behaviour should not be too tightly associated only with the Materials Panel - it is an essential area for development across many disciplines.

## 1.2 Materials and Foresight: the rôle of modelling

### General observations from Technology Foresight

The overall report on Technology Foresight [OST 1995a] made a number of observations on the state of UK science and technology. Many of these were strongly endorsed (or qualified somewhat) in responses from (for example) the Royal Society. Some pertinent general comments are as follows - all of which could be held to apply to a significant degree to materials modelling:

- British science is excellent, while in comparison its record of exploitation is poor.
- UK international competitiveness is largely driven by advances in science, engineering and technology
- it is vitally important to maintain a strong science base, and to support very good work (without excessive regard for whether it matches the Foresight objectives).
- technological literacy of senior managers tends to be low; similarly business literacy of scientists and engineers is often low.
- frequent interaction between science and business communities about trends in markets and technologies is essential.
- networking and communicating technical advances to smaller companies is very important.
- inter-disciplinarity and multi-disciplinarity should be encouraged rather than forced. Incentives for collaboration (e.g. earmarked EPSRC funding) must be flexible.
- collaboration with EU partners is of great importance.

### Sector highlights

The general Foresight report [OST 1995a] summarised each Panel's reports via "sector highlights". A number of these are summarised below, to further identify themes and contexts which should be considered in terms of their impact on materials modelling.

The central rôle of materials modelling is self-evident in Materials, Chemicals, Transport, Defence & Aerospace, and in Manufacturing, Production & Business Processes. Energy and IT & Electronics each highlight developments, primarily in functional materials, in which modelling can be assumed to play a part. Three other sectors (Construction, Food & Drink, and Agriculture, Natural Resources & Environment) all have a strong materials element, but it is not clear whether modelling has been considered sufficiently by these Panels. A few remarks are therefore added on these sectors.

## *Materials*

- high-temperature and weight saving materials; sensors, modelling, biomaterials, superconductor processing (as noted above)
- competitive advantage is most likely to come from continuous improvement in existing materials and processes, and commercial exploitation of existing materials in new areas
- integration of materials science and modelling with product design; concurrent engineering/rapid prototyping

## *Chemicals*

- synthesis, processing and structure-property relationships of materials, especially polymers

## *Transport*

- vehicles with greater efficiency and reduced environmental impact (weight-saving materials)

## *Defence and Aerospace*

- process technologies, simulation and modelling, materials and structures - all key priorities
- rapid growth of civil aerospace markets, dominated by need for lower manufacturing costs and reduced time-to-market

## *Manufacturing, Production and Business Processes*

- management gives insufficient coupling between technology and marketing
- R & D too remote from market, too low a proportion of turnover, or only conducted for very short-term payback
- technology priorities: processing plant development, sensors and controls, modelling, simulation and visualisation of processes, materials processing technology (including joining)

## *Energy*

- materials for photovoltaics, and fuel cells

## *IT and Electronics*

- semiconductor and display materials

### *Construction*

The emphasis in this sector is on the built environment and customisation in construction. Construction materials are not given much prominence, which in view of the economic importance of building materials (including roads), could be regarded as something of an omission. Greater consideration is merited for scientific research into processing and/or performance (especially the effect of environment) of cement, concrete, asphalt, bricks etc. The potential of modelling in this area is considerable, and largely untapped. A report to EPSRC on materials processing also highlighted construction materials as a neglected but very significant area (Hollox [1993]).

### *Food and drink*

Food production in many respects resembles a large, complex materials processing industry. Foods are composite materials on many different length scales. Modelling of food processing is a major activity in some food producing companies, though the knowledge and techniques used can be very proprietary information. The potential of a greater exchange of process modelling expertise between the food processing sector and the materials science and engineering communities does not appear to have received enough attention to date in Technology Foresight.

### *Agriculture, Natural Resources and Environment*

Several materials themes were noted in this sector:

- environmental policy can be a major driver for reusable, recyclable and other novel materials and products, efficient power-producing plant and transport
- greater emphasis is needed on sustainable resourcing of materials - particularly in construction
- substitutes will be required for materials legislated out on environmental grounds
- improved technologies are required for using forest products

Modelling does not have such an obvious direct rôle here, but these themes nonetheless emphasise some of the emerging changes in perspective in materials research. Modelling of materials processing or performance as a direct or indirect consequence of an environmental issue is an activity which can be expected to increase.

## The Materials Panel Report

### *General points*

Many of the main points to emerge from the Materials Panel have been summarised already, but the report of this Panel [OST, 1995b] clearly merits more detailed consideration. Two general matters were raised, which also emerged as recurring themes in this review:

- modelling brings with it the need for good data
- UK education and training in materials science/technology is wanting

The Panel recommend that the training of materials scientists should include 2 years of basic science and engineering, and 2 years of specialisation, with greater industrial relevance throughout. Education for materials modelling was not directly addressed, but perhaps should have been given the prominence of modelling in the overall recommendations. This raises many issues in its own right (Sargent et al. [1993]), and will be considered further later.

The needs for education and training extend beyond university courses to industry and academia as a whole - there is a need to change attitudes between industry and academia and to aim for the provision of technically competent trained manpower at all levels.

### *Structural and functional materials*

Some distinctions between structural and functional materials were drawn:

- microstructure and composition are critical to understanding processing and performance in structural materials
- new structural materials don't create new products, but may enhance existing products; the emphasis should be on improving the materials already in use
- applications of functional materials are more device-based - less dependent on the detailed physics of the materials within the devices
- new functional materials (or devices based on them) do rapidly lead to new products (e.g. laptop PC, mobile-phone)

There will of course be exceptions to these statements, so they shouldn't be taken too far, but they again provide a focus for a review of modelling needs. This review concentrates on structural materials, as it is judged that the industrial context of functional materials is so different. The Panel commented that few UK companies are able to exploit the developments in

making devices and thereby attract inward investment, so the recommendations for development were less conclusive in this area. A separate study of materials modelling in this field is strongly recommended, which could include consideration of the benefits of stronger links between the structural and functional materials modelling communities.

### *Delphi Survey and Regional Workshops*

The Delphi survey appears to have made almost no impact on the discussion of materials modelling - the questionnaire did not particularly invite input on modelling, and only produced one specific response on molecular modelling. The prominence of modelling in the final recommendations was clearly not a consequence of the survey.

A few of the points raised merit comment in this context:

- there was broad agreement that collaboration within UK and Europe is necessary to meet Panel targets. This is absolutely the case in the context of modelling, though some argue that *worldwide* collaboration is more accurate.
- the UK was reckoned to be a leading edge country in various materials areas including modelling of life prediction. Process modelling was not mentioned, but there is no reason to suspect that the UK is lacking in this area.

The Regional Workshops gave greater emphasis to materials modelling, with discussion of themes such as: intelligent processing; modelling linking "craft wisdom" to science in materials processing; measurement and modelling needs for control. Modelling of processing emerged as vitally important for the future of all classes of materials.

### *Classification of R & D needs*

The Panel classified R & D needs under various headings. Those relevant to materials modelling are summarised below, with comments.

#### **Generic topics**

- microstructure and composition are critical to understanding processing and performance in structural materials
- continuous development of existing materials; in the past this has not been widely popular with universities and funding bodies, but this situation is changing.

### Computer-based underpinning techniques

- theoretical screening to determine optimum compositions (materials science aspects): potential across all length-scales from atomistic to phase diagram calculation to microstructure-property prediction; parallel computing essential development for some of this work.
- principal thrusts: reduced trial-and-error in experimental work, faster/cheaper material development.

The success of “computer screening” in developing drugs is much cited, but the analogy with engineering materials should not be carried too far, where there is a different complexity of hierarchy in microstructural length-scale - this is discussed further later.

- process modelling (materials engineering aspects): needed across all manufacturing industry (raw material extraction, forming, fabrication, machining, surface engineering); high quality data measurement and metrology capability needed (and in danger of being eroded); links with design process important.
- principal thrusts: improved quality and consistency (at least as important as mean properties), reduced lead times and manufacturing costs.

### Related underpinning techniques

- sensors - interaction with modelling community needed to build models with realistic potential for using on-line measurement
- testing and evaluation - data needs of manufacturing are very large (and should include the needs of materials modelling)
- joining technology

The approach to joining is very "techniques" based (perhaps reflecting the research emphasis of TWI). The potential of modelling both processing and performance in joining was not highlighted, but should not be overlooked.

### Specific topics and emerging areas

No particular reference was made to modelling in these areas, but it comes into all as an underpinning technique:

- higher temperature materials
- weight-saving technologies
- IT and telecommunications
- biomaterials
- controlled molecular architecture polymers
- high  $T_c$  superconductors: processing now the priority
- functional materials

## *Findings and recommendations*

The Panel summarised the key aspects for materials as follows:

- improved performance of systems and products limited by materials in many sectors (aerospace, automotive, power plant, offshore, telecommunications)
- incremental improvements by better processing (modelling, sensors, control)
- reduced government laboratory R & D in materials - increasing role of universities
- degree level teaching of materials science in need of review
- collaboration with (at least) Europe is essential; largely multi-disciplinary work needed
- worldwide science watch essential (the Royal Society response to Foresight also emphasised that technological advance can come from anywhere in the world)

## *Implementation*

- Institute of Materials to contribute to establishing collaborative partnerships
- universities to catalogue and disseminate information from UK and rest of world by electronic media
- EPSRC shift of funding towards continuous development of existing materials, and away from breakthrough areas; new Managed Programmes to carry Foresight objectives
- strong industrial involvement, and increased technology transfer to SMEs.

The position of industry needs careful consideration in the area of materials modelling. The Panel proposes that industry must lead in specifying opportunities, needs etc. This general position does not entirely hold in modelling - it is only appropriate for modelling-literate companies, who are predominantly the large companies. It can't be expected that industry will take the lead in implementing modelling and directing research effort, when a great deal of industry is unaware of the potential benefits. Rather the universities and national centres with modelling expertise need to draw the industrialists in, via collaborative research, taking the lead from the much greater industrial application of modelling overseas, particularly in Japan.

This type of technology transfer requires careful handling, particularly for SMEs. Modelling is all too easily oversold - software which fails (or disappoints through unrealistic expectations having been built up) potentially sets back the uptake of computer-based methods another decade for that company. As in most technology transfer, the transfer of people is the best way forward: by recruitment, secondment, frequent meetings etc. Personal interaction and the ability to represent Foresight concepts in an industrially relevant manner were seen as essential by the Materials Panel. This is particularly challenging in modelling, which often has an aura of mystery to non-academics.

## **Working Party on Aerospace Structural Materials**

One of the first responses to Foresight from the Institute of Materials was the report for the Materials Strategy Commission by a Working Party on Aerospace Structural Materials [Institute of Materials, 1995]. The report documented key materials and processes expected to develop over the next decade - similar sector surveys will doubtless continue under Foresight.

Materials developments in which modelling was regarded as critical were:

- development of Ni and Ti alloys
- processing, design and performance of polymer matrix composites (aircraft structures, and helicopter fuselages)
- development of surface treatments and joining techniques

The Report noted that high quality expertise for aerospace materials is available in the UK (including modelling) but it is thinly spread. Centres of Excellence are preferred, with teaching links between industry and the selected universities. How modelling fits into a system of Centres of Excellence will need to be addressed - this is discussed further later.

## **EPSRC response**

The EPSRC Programme for 96-97 [EPSRC 1996a] demonstrates considerable resonance with the outputs of the Foresight exercise. The importance attached to modelling and simulation by EPSRC is clearly stated in its own response to Foresight [EPSRC 1996b]. For some reason in the final Table of EPSRC's response "modelling and simulation" as a topic area is not linked to the Materials Programme, which one can only assume is an oversight.

The EPSRC Materials Programme was also influenced by its own earlier survey (Hollox [1993]), which gave a more detailed appraisal of the UK materials processing situation. Not surprisingly, many of the Foresight recommendations overlap with the findings of the earlier report. Hollox particularly mentions:

- continued support for casting, to exploit new-found maturity
- forming processes (especially forging)
- surface engineering
- joining
- polymer composites processing
- in-process control methods
- building materials

It was also emphasised that conventional materials (for which processing costs are critical) required far more attention, and had been over-shadowed by novel (expensive) materials. It was suggested that the necessary shift could be achieved by managed programmes, while leaving room for responsive "blue skies" research. Managed programmes discussed in the current EPSRC Materials Programme are:

- Processing of Conventional Structural Materials (the first round of which starts shortly) - with the emphasis on improved consistency and performance, lower costs and minimisation of environmental impact.
- Predictive Modelling of Materials - with the emphasis on multi-scale modelling, or linking materials composition, structure, process parameters and end product performance (considered in May 1995 at a discussion meeting, but not yet taken further)

The other themes highlighted by the Materials Panel are covered by the responsive mode, with much of the activity also falling within the remit of the materials IRCs.

Several other EPSRC Programmes have an interest in materials manufacturing and performance, and support modelling work:

- Design and Integrated Production (DIP): materials process modelling is a continued major thrust of the Manufacturing Technologies theme; initiatives are planned in processing of materials to produce near net shape products.
- Innovative Manufacturing Initiative (IMI): aerospace sector closely involved with low cost composites manufacture; high temperature and low weight materials; rapid product design.

There is further overlap in materials modelling with the Process Industries sector of IMI, the Process Engineering Programme, and the Mechanical Engineering Programme.

Materials modelling therefore emerges as an underlying theme within EPSRC, particularly in new initiatives. It appears undecided as to whether a modelling initiative will emerge in its own right or whether modelling will receive "favoured status" within other programmes. The latter has much to favour it, as it encourages keeping modelling in perspective, and promotes multi-partner projects or suites of projects at a single institution (such as an IRC), where modelling and experiment can run in parallel. There is otherwise a danger of generating a modelling bandwagon, with too much emphasis on modelling techniques, and insufficient guidance from real end-users.

Finally, it is worth commenting that EPSRC could have a role in *training* for modelling, since education/training repeatedly emerges as a critical factor. Consideration should be given to materials modelling within the EPSRC training initiatives (e.g. one week graduate schools, Engineering Doctorates, Research Masters, the Integrated Graduate Development Scheme, the Teaching Company Scheme, or Faraday Partnerships).

## **Foresight Challenges in Materials**

The first direct funding initiative in response to Foresight was the Technology Foresight Challenge Competition, funded jointly by the DTI and industry. Of the 24 new projects, two are in Materials and have modelling as a central theme. One project plans to use computer modelling to design new materials for turbine blades, initially targeting aerospace, but later considering the power generating industry. The second project aims to develop computer modelling for the polymer industry, particularly aiming to take modelling from the chemistry level into the meso-level, to give greater industrial relevance. Both include hierarchical modelling as a major theme, but the scientific challenge is to identify the most critical connections to be made for the particular class of material and behaviour in question.

## **European dimension**

Collaboration in Europe may be conducted by direct industrial/academic links, or through major EU-funded programmes (though many are deterred from these by the volume of paperwork in making proposals and running projects). Most UK industry will not hesitate to go to a European university to collaborate if expertise is insufficient in the UK; similarly it is essential for UK universities to be looking to European industry. Some academics feel that industrial collaboration in Europe does not gain sufficient recognition - either in current competition for funding, or in the Research Assessment Exercises.

Many of the targets of Technology Foresight in materials modelling may be found in the goals of the 4<sup>th</sup> Framework programme, and can be expected to continue in the new 5<sup>th</sup> Framework programme from 1998. There have been a number of dedicated European programmes in materials modelling and processing. COST 512 (Modelling in Materials Science and Processing), which finishes in summer 1997, consists of 55 projects covering almost all the modelling areas discussed in this report [Rappaz and Kedro, 1996]. British involvement in this programme was less extensive than might have been hoped, though more specific programmes under ECSC or Brite/Euram (e.g. in hot rolling) have involved the UK material suppliers and universities.

# Materials modelling: General issues and needs

## 2.1 Introduction

This section addresses the general issues in materials modelling. It draws on the interviews conducted and questionnaires received during this study, but also on an updated interpretation of the report by Sargent et al. [1993], on Modelling Materials Processing for the ACME Directorate. In addition, the unpublished SERC report by Hollox [1993] on Processing and Engineering Application of Materials, has been consulted (courtesy of EPSRC) and the modelling implications of that study incorporated as appropriate. More detailed consideration of particular materials and process sectors is given in section 3.

## **2.2 Overview of issues in modelling materials during processing and in service.**

There is a world-wide consensus that a group of disparate disciplines (materials science, mathematical modelling and computer science) have evolved simultaneously to a point at which a new synergy is possible. The potential of materials modelling and simulation appears to be very considerable, both in terms of economic gain, and in terms of gain in performance, safety and environmental protection. Investment in this area is high in the USA, Japan and Europe, and so it is entirely appropriate that it emerged as a key area from the Technology Foresight exercise.

In all problems of materials processing and performance, the number of variables is large - often far too large for a purely empirical approach to be commercially viable. The appropriate use of physical understanding reduces the number of independent variables, or at least couples and constrains their variation. This is an essential step to providing predictive capability, which should be the ultimate purpose of any modelling activity.

### **Interpretation of "materials modelling"**

Materials modelling can mean many different things to people, so it is necessary to define what is meant by the phrase here. For the purpose of this report, materials modelling implies:

- linking processing conditions to properties and performance
- linking service conditions to performance and failure

Processing and service conditions should be taken to include idealised laboratory conditions and tests, as well as the real manufacturing process or application. The links may be made directly (constitutive modelling) or via a description of the material at some level of microstructure below the continuum (physically-based modelling).

The term "modelling" is also commonly used to cover empirical methods, including advanced statistical or knowledge-based approaches such as neural nets, fuzzy logic or expert systems (in which physical knowledge may also be embedded). Not everyone is happy with this breadth of the term "modelling", but it is inevitable as the boundaries are becoming less distinct.

Neural nets and fuzzy logic are best applied to problems with large amounts of empirical data. In many areas of processing or performance, the underlying science is well understood and characterised for idealised

materials and laboratory conditions. The difficulty in generating reliable quantitative predictions comes from the inevitable complexity in commercial compositions, in combination with real process or service histories. The neural net and fuzzy logic approaches appear well-suited to investigating these problems. A hybrid approach is to embed what reliable physical correlations there are into the neural network. There is a very different ethos in implementing these techniques for multidimensional data interpretation, which can appear to undermine the need for fundamental scientific understanding. It is important to keep the methods in perspective, but the most exciting research may well emerge from groups which simultaneously develop physically-based models and statistical methods.

Most of this report relates to modelling of the constitutive or physically-based variety. This includes fluid flow, thermal analysis and continuum and damage mechanics (primarily by FE analysis), and physically-based microstructure modelling.

### **Modelling processing and modelling performance**

Some distinction can usefully be drawn between modelling material processing and modelling material performance - though much of the purpose of modelling is to predict the connections between the two, and they draw to a large extent on common underlying materials science. Process modelling originated in chemical engineering, predominantly concerning processing of gases and liquids. The challenge for engineering materials is much greater, involving liquid or vapour transitions to the solid state, and great complexity of solid-state behaviour. This requires a combination of engineering science (fluid flow, heat flow, plasticity) with materials science (thermodynamics and kinetics of microstructure evolution, and microstructure-property characterisation). Its focus is not just the resultant properties of the material, but includes control of the process and maintaining quality during processing, and the design of processing equipment itself. There is also an increasing need for the integration of processing knowledge into product design.

Modelling for service is aimed at understanding failure mechanisms, and integrating this knowledge with engineering design. There is a parallel growth in the interaction between engineering disciplines (continuum mechanics, fracture mechanics) and materials science (microstructure evolution under load, in some cases incorporating the effect of a hostile environment, or high temperature service). Modelling for service mainly aims to provide lifetime prediction under conditions of corrosion, wear, creep, fatigue, or high velocity impact. This enables design codes to be less conservative, often leading to a more efficient use of material and reduced weight and cost.

One aspect of this survey has been to investigate the balance of activity between processing and performance in the major material classes: metals, polymers, ceramics and composites. This may be summarised as follows.

### *Metals*

- greater emphasis now on processing than service
- some sectors believe performance modelling (e.g. vibration, stress and thermal analysis) is greatly over-worked relative to processing
- linking processing through multi-stage processing, and linking processing to performance explicitly are major emerging modelling challenges (e.g. residual stress, composition and microstructure)

### *Polymers*

- processing dominates constitutive modelling
- physically-based modelling for prediction of properties (both for processing and in service) directly from molecular behaviour becoming mature
- major growth in linking composition, microstructure and stress state from process through to performance

### *Ceramics and Composites*

- ceramics: mostly constitutive modelling of processing
- composites processing - traditionally little modelling input, but some potential in the push for low-cost manufacturing routes
- composites performance - damage mechanics very extensive at test coupon level; major challenge to transfer expertise to component level and real design.

## **Appropriate modelling**

One of the greater challenges which emerges from this review of materials modelling, particularly for metals and polymers, is linking the hierarchy of microstructural length-scales which determine the macroscopic properties of a material during processing or service. Closely related to this is the range of time-scales on which microstructural phenomena occur. Modelling skills exist at all levels, and there is great scope for making connections between length-scales and time-scales. It is essential however that the appropriate level of complexity is adopted for any modelling exercise. If the "next step" includes an identifiable need to link different scales, then this is an appropriate challenge to take up. Forging links without a clear goal for doing so can otherwise become a purely academic modelling exercise.

A related general aspect of materials modelling is that the modelling skills and innovative thinking required for progress are strongly influenced by the purpose of the modelling activity, and the background of the modeller. Academic materials scientists and engineers seek to base models on fundamentals - thermodynamics, kinetics, micro-mechanics etc. From an industrial perspective, the underlying science is secondary to the provision of a useful tool: many industrial models contain no science at all. There are enormous gains to be made by bringing these views together in a careful blend of both science and empiricism. On the one hand, this could imply the steady development of physically-based but industrially useful models. On the other, it could mean exploitation of the more sophisticated empirical techniques such as artificial neural networks.

Modelling for industrial relevance is not anti-science: in most fields, modelling stimulates research in the underlying physical processes. Not all modelling needs to be commercialised to be deemed successful - good "research models" are of great use to the research and development community, even if they never find their way into end-user packages. Eventual industrial application should not be the only yardstick with which to measure the value of a materials modelling project.

## **Aspects of collaboration in materials modelling**

### *Academic collaboration*

Research in materials modelling requires three essential components: mathematical methods, materials science and computer/software science. This is not always recognised in research proposals, which must however demonstrate that the full range of expertise is available. This is now rarely true of one person or even a group (except perhaps for supporting experimental activities). Collaboration is therefore essential, and this is now largely recognised by funding agencies. It has been commented though that in the UK academic appraisal and the Research Assessment Exercises (RAEs) perhaps still over-emphasise individual activity.

Properly defining the problem is crucial - this requires a close interaction between end-user and scientist. Many university/industry links are too narrow, simplistic or remote, and are not always well-supported by current funding arrangements. More basic research in industry, and more serious involvement of universities in application are needed, as achieved in other countries. Some of the EPSRC schemes (such as the Teaching Company scheme) are a step in this direction.

It has also been commented that a lot of the best materials scientists with real physical insight are essentially experimentalists, with little or no interest

in embedding their knowledge into research software - even less into commercial code. The reverse is also true - many mathematicians and software experts have a very sparse knowledge of materials science.

Research which aims to produce software for industry must also ensure that such software is properly packaged and validated. The former ACME Directorate, which became part of DIP in EPSRC, monitors projects more closely than most to try and see that this is achieved. Collaborative projects between materials and computational experts might be enhanced if projects were jointly funded, so that both groups are properly supported - this is not easily achieved in the present funding structure. It also implies that funding for process modelling research must recognise the need to include the cost of programmers. This leads on to the often thorny questions of deliverables, commercialising software, IPR and so on.

#### *Collaboration within industry*

In modelling manufacturing processes, a further spectrum of skills is required to complete any modelling task: from people close to the product design and the manufacturing processes, who understand the business context of the problem, to those with computational and scientific skills to implement and test the models. Historical factors mean that, in the UK (and probably elsewhere), there are often significant cultural gaps between designers, modellers and machine operators. This raises the issue of education and training, which is discussed later.

Even if all the relevant skills are available, it is critical that the correct modelling infrastructure is supported for modelling to be effective and used routinely. It should also be recognised that implementing and using a modelling system within a manufacturing system provides opportunities to productively enhance the structure and dynamics of the latter.

In any industrial sector or individual company it is therefore important to address the current position with regard to modelling. Is the challenge to inform and train industrialists in new computer-based technology? Is it to improve the productivity of existing modelling, by developing techniques and improving data? Can modelling be better integrated with the overall structure of the manufacturing system? Are there fundamental gaps in underlying scientific knowledge of the materials behaviour in question? Academics and research organisations have a role to play in all of these, but greatest emphasis needs to be given to transferring existing science and technology to industry.

## A structured view of materials modelling

Developing predictive models for materials processing or performance in order to optimise a material, a process, or a design is greatly enhanced by taking a structured view of the problem (Sargent et al. [1993]). This is true in two distinct ways:

- understanding the underlying materials and engineering science at the appropriate level of detail [Ashby, 1992]
- understanding the software engineering implications in constructing, validating and maintaining computer code [Wood, 1993a]

A previous study of modelling materials processing [Sargent et al. 1993] started from the hypothesis that much of the value of modelling research is lost, since the models are developed and validated for a specific problem, whereas much of the modelling activity is generic. The review discussed this in relation to data manipulation, model building and efficient software engineering, so these aspects are not considered further here.

A second hypothesis underlying the earlier study was that inappropriate modelling techniques are too often used. Numerical methods are often used when really only qualitative results are required. Finite element modelling in particular is a notoriously all-absorbing activity. There is still a clear need for a systematic means of *classifying* modelling problems in terms of the process physics and solution techniques, and this is an essential feature of training both model developers and model users. The key ideas from this second generic aspect of modelling are incorporated below.

## 2.3 Modelling: what is it for ?

From the manufacturing engineer's perspective, modelling can serve many purposes (Sargent et al. [1993]), all in some way related to a commercial need:

- to optimise an existing process and improve productivity
- to improve quality by reducing product and process variability
- to reduce the number of trials in developing a new or modified process or product (rapid prototyping, shorter design cycles)
- to improve process control systems - "intelligent processing"
- to improve management of production schedules
- to improve the manufacturing capability of suppliers to larger assembly companies
- to aid development and specification of new equipment and tooling
- to gain knowledge and education (visualisation, process parameter studies, scientific explanation of observed phenomena)

Enhanced process visualisation and understanding is a difficult benefit for a company to quantify. Many industrial modellers firmly believe however that this is an essential function of a process modelling group. The dialogue between plant operator and modeller encourages a more questioning view of what must be controlled to maintain product quality. Improved productivity can result simply from this exchange, even if the subsequent simulation is never fed back to the plant.

In certain sectors (notably safety critical jet engine manufacture), knowledge of process modelling is a critical part of Quality Assurance. Suppliers must show that they have validated models of their own processing in order to win a contract - modelling can therefore play a key role in attracting business. This can be expected to steadily expand to other sectors.

Commercial software for materials modelling is in itself a marketable product leading to direct wealth creation from sales, licences and user-support contracts. While UK companies should of course aim to be strong players in this field, the significant wealth creating potential of modelling comes from its use by industry, not from software sales.

## **Integration of processing into design, and product tracking**

Two very important themes emerge from this survey:

- integration of processing into design
- tracking the state of a product through multi-stage processing, and from process into service

Concurrent Engineering and Design for Manufacture are popular current manufacturing topics, in which modelling can play a major role by bringing processing information efficiently into the design process. For example, approximate "short-cut" FE stress analysis may be directly integrated with CAD, offering great gains in efficiency by reducing the need for so much detailed stress analysis later on. Much the same may be said of running simple process models (e.g. for casting) directly on the output of CAD, as this allows screening and modifications of a design at an early stage. An added benefit is the way that simulations allow not only modification to designs to take account of processability, but enable efficient co-selection of alloy and process (including the potential for optimising compositions).

Tracking of product state (either its microstructure, or its residual stress state) is also an area ripe for development. Research is needed on how to capture these essential characteristics for subsequent modelling of behaviour. An important aspect of this is to note that models may then

need to incorporate features which play little or no role in the current step being modelled, but which can be critical downstream.

Downstream processing steps or service are most often in the hands of another company. Software is also increasingly used as the routine means of communication between customer company and suppliers. Industrial modelling thus requires a shared understanding of the purpose and capabilities of the modelling between supplier and customer.

These developments imply a growing need for reliable software to feed forward the output, either from CAD to process simulations, or from a process simulation into subsequent stress analysis or the next process downstream. Links between CAD - FE mesh - simulation - visualisation of process all need to be more robust. This approach has strong implications for how software is constructed at each step, with a need for greater coupling up and downstream, and much more automatic data transfer from stage to stage.

### **Modelling of standard tests**

Modelling in industry has a role beyond simulating actual manufacturing processes - it is also a powerful tool for modelling the standard tests used extensively to characterise material constitutive behaviour, effect of composition, boundary conditions and so on. Modelling mustn't stop here, or the benefit to the real process or component can be quickly saturated. Many standard tests have long been assumed to be homogeneous - modelling allows close interrogation of thermal or deformation gradients which have hitherto been hidden. It also allows sensitivity analysis on how carefully the tests are conducted, e.g. variability due to (for example) changes in friction conditions. It is often the best place to start for modelling the effects of composition, since some of the complexity and uncertainty of the behaviour in a real component are removed, and the test itself can be very well-understood for a number of standard compositions.

### **Modelling versus experiment**

The usefulness of a model can only be assessed in comparison with other ways of estimating the same information - usually handbooks and the judgement of experts, or experimental trials (Sargent et al. [1993]). Models are not necessarily cheaper or faster than performing a real experiment. The ability to recognise tractable from intractable problems is very valuable, and some of this can be taught.

The asymmetry in information between simulation and experiment is also very significant. For example, a shaped casting thoroughly instrumented with thermocouples is more expensive than a simple trial, but a model can display results with “virtual” thermocouples everywhere. A trial casting will show the location of porosity but its microstructure gives little information about the conditions which led to the porosity.

### **Simple models and whole process models**

Quite coarse models are appropriate for modelling entirely new processes or where an established process is to be scaled up or applied to a different material. Simple models can be condensed into process diagrams, or simple software, and provide first estimates for trials which will then be tested empirically. Significant savings can be made just from getting an improved first “guess”.

Improving the understanding of an existing process may require a more complex model. Improving quality by reducing variability nearly always requires second order effects to be taken into consideration. This also requires a greater range and detail of experimental data to provide model parameters and validation tests. “Deep physics” models have a role to play, but tend to get bogged down on the detail of one difficult physics problem. This is all very well from a scientific viewpoint, but sooner or later this knowledge needs setting in the context of the overall process.

“Whole process models” are rarely attempted, so the genuine and unavoidable complexity of real problems is avoided. This can lead to lost opportunities - for example, in the development of models which link composition to properties, processing and performance (as advocated strongly by the Foresight Materials Panel). A partial picture of these links could result in models which, for example, predict optimum composition from the point of view of properties, but which could not in practice be processed. Some attempts to link composition to processing and final part properties stumble for lack of good microstructure models. Pragmatic modellers use empirical relationships to see the job through, and this is a creative way of highlighting the more fundamental studies which are needed.

“Reduced modelling” is essential from the start. Industrial application cannot wait for an eventual complete model that covers everything from atomic interactions to microstructure, properties and residual stress. It is more important to deploy some simple models in practical situations so that later, improved models have a route to application. For the most complex processes, this may simply be a database of treatments, organised using

simple analytical tools (such as dimensional analysis and approximate heat flow, plasticity etc).

Intelligently deriving a simplified model from a complex model is a difficult modelling challenge, requiring real insight in choosing what to leave out, and how to make approximations. It is hardly ever done in practice - in spite of the obvious benefits of doing so. This probably reflects the quite different modelling ethos and skills needed, compared to devising the complex model in the first place.

### **Sensitivity analysis and validation**

Sensitivity analysis in all materials modelling is absolutely essential. It identifies where modelling effort should be concentrated, the appropriate degree of precision, where data gathering should be concentrated, and the confidence level of the predictions. Increased computer power is however almost always absorbed in more complexity instead of more runs of an existing model, exploiting the increased speed. This is particularly true in FE analysis, with a few notable exceptions. A guiding principle advocated by some experienced modellers in academia and industry is that models should always operate one step behind the current possible complexity.

A simple version of a model run many times to indicate the sensitivity of the output to variability in the input is frequently of much more use than a single complicated computation using the "best" estimates of the materials parameters. Studying the effect of varying one parameter at a time is a quick but limited way of observing sensitivity in a model. Non-linear systems should strictly be tested using a Taguchi-style matrix of sensitivity experiments. Many models in the literature have clearly not been thoroughly "interrogated" - if at all.

An important type of sensitivity analysis is evaluating the sensitivity of the product state (properties or residual stress/distortion) to poor equipment set-up (rolls out of parallel, worn dies, lubricant breakdown, poor temperature control etc.). This type of analysis is where very direct modelling benefits can occur, simply by raising the awareness of the machine operators as to the consequences of what they are doing, as noted above.

What is considered to be appropriate validation and sensitivity analysis can also mean different things depending on your point of view: e.g. validation of predicted properties, or validation for better process control during processing? Validation must therefore be fit for purpose.

Validation is absolutely essential to convince industry that a model is worth having - a model must at least demonstrate that it can predict what they

know already. Insufficient validation is done largely because it is an additional cost in the project which can appear unnecessary, and it is a much more repetitive and a less absorbing challenge to the modeller. The same can be said of conducting proper sensitivity analysis, which is equally important.

It is encouraging to see the high profile given to sensitivity analysis in one of the NPL co-ordinated projects within the DTI Processability Programme on Liquid Metal Processing [NPL, 1996].

## **2.4 Modelling: identifying what is important**

Sargent et al. [1993] discussed the computational aspects of industrial process modelling in some detail. Many problems cited in that report have since diminished (e.g. slow automatic remeshing), and can be expected to become routine in due course.

The emphasis in this report is not the computational aspects of materials modelling, but it is worth restating that too little computing expertise is generally brought to bear on materials and process modelling activity. The converse is also true - some mathematically and computationally skilled groups undertake materials modelling with inadequate knowledge of materials science. No amount of computing power compensates for poorly understood physics or metallurgy.

### **Choice of modelling method**

One of the most important aspects is deciding on the appropriate modelling method for the problem concerned. Appropriate does not mean using the most complicated currently available, especially in the context of Foresight where the aim is to get academic work to be of greater benefit to industry. The focus should be the process or phenomenon itself - not the modelling technique. Development of techniques should be clearly justified by examples of the intended application - otherwise this can be left to the mathematics community. Most modelling tools are now sufficiently developed. Decisions on funding materials research should be made primarily by people whose main interest is in materials, not computer methods. At the same time, the increasing popularity of modelling should not be allowed to develop into a research bandwagon.

The choice of modelling technique should justify the level of complexity - as noted above, some say that over-elaborate software is being used almost all

the time. It is reminiscent of the endless trend in word-processing and other desktop software - for every order of magnitude increase in the MBytes of software, most people probably use less than double the complexity of what they were doing before. A culture of working up through a modelling hierarchy of steadily increasing complexity, as required by the problem in hand, is urgently needed.

Analytical techniques can be very powerful and fast - to map out the full parameter space, to identify key parts of the problem, and thus to focus numerical methods and experiment. There are some useful guidelines as to when it is adequate to use analytical algebraic equations and when it is necessary to construct a discrete meshed model, e.g. for finite element or finite difference calculations. It is always necessary to do some non-meshed modelling in order to decide on appropriate boundary conditions for the meshed part of the problem. FD and FE solutions for real geometries are now quick enough for on-line use, but have so far not been exploited for microstructure prediction and informed sensitivity analysis.

There are only four reasons why a numerical meshed method might be appropriate:

- the modelled volume has some complex shape
- the modelled volume contains numerous internal structures
- the modelled volume contains discontinuous behaviour
- the underlying process physics are very non-linear (either within the material or in the boundary conditions)

These are difficult issues, as discussed by Sargent et al. [1993]. Complexity of geometric shape may not lead to complexity in the underlying physics (such as heat flow). This is often a matter of distinguishing between surface effects and bulk effects, and giving careful attention to the length scales and time scales controlling the underlying physical phenomena. In the same geometry the complexity may also vary from material to material - e.g. depending on the thermal conductivity, heat may travel a small or large distance during the process compared to the size of the component.

Another distinction between analytical and numerical methods arises due to transients. In some processes there is an important initial and final transient, which requires numerical techniques, with only the long "steady-state" in between being simpler to model and amenable to analytical methods. Consideration needs to be given to where the dominant problems lie, as these are often in the transient regions. Examples are the initial threading of coils in strip rolling, or the transient heat flow at the start of welding.

Analytical methods and numerical methods should therefore be regarded as complementary, and a proper awareness of both should form an essential part of training model developers and model users. It should never be a case of "use the FE package because we've got it".

## **Boundary conditions**

Determining the boundary conditions of a processing problem is a major part of the activity of process modelling (Edwards and Endean, [1990], Sargent et al. [1993]). Boundaries are not just geometric shapes, they are also statements of symmetry and continuity with respect to time, or variations with respect to other parameters such as temperature. Interface phenomena can prove a very difficult aspect of process modelling, as many interface parameters cannot be measured directly. This implies a need for alternative approaches to the problem, such as experiments combined with inverse analysis, or modelling of the interface as a micro-process in itself.

Analytical solutions are heavily constrained by boundary conditions, numerical methods less so, but the type of numerical solver is strongly influenced by the complexity of boundary conditions in the problem. Therefore intelligent use of numerical meshed models requires intelligent selection of numerical analysis techniques, which typically reduces to the selection of a particular software package (and solver algorithm). This also has implications for education and training, and also for guiding the development of software appropriate for the end-user.

## **Classification of modelling**

Major parts of any modelling task are deciding:

- what is the physical behaviour being described, and what is the scope of the problem?
- what modelling methods and software implementation are appropriate for this problem?
- what experimental support is required for input data (bulk properties and boundary conditions), and for validation of the output?
- what predictive capability will the model then provide?

In view of this, Sargent et al. [1993] concluded that there was a need to classify materials processing in relation to modelling techniques, and proposed a tentative approach to doing this. Conventional classifications by type of process (Edwards and Endean, [1990]; Lenau and Alting, [1988]) are limited in the guidance they give to selecting modelling method. For example, from

the modelling point of view, friction welding has as much in common with forging as it does with arc welding.

Many of the modelling and software problems are very similar in casting, forging, extrusion etc. - e.g. 3D CAD geometries, complex flow problems, coupled internal heat generation, deformation and heat flow, and complex heat transfer at the boundaries. Polymer moulding and metal casting also share many underlying problems. There is therefore great potential for technology transfer between widely different processes (and materials) which are not necessarily linked in most people's view.

The approach to modelling proposed by Sargent et al. has some potential as a basis for the education and training of modellers. Many of those consulted in this study regarded the principal requirement in a modeller to be one of outlook and attitude, i.e. an open-minded approach, a gift for lateral thinking, and a clear view that a model is a tool to reach an end rather than an end in itself. The classifications proposed encourage this way of approaching modelling.

A classification of processes from the modeller's point of view thus potentially serves a number of purposes:

- as a guide to identifying the appropriate modelling methods for the problem in hand - the type of prediction required strongly influences the type of model needed (e.g. field variables only, or microstructure, or defects)
- as a means for improving the rational allocation of resources between and within modelling projects, both in academia and in industry
- as a mechanism for integrating the different approaches to modelling
- as a basis for training modellers with an open-minded outlook, encouraging innovative thinking

## **2.5 Data for Materials Modelling**

Everyone involved with real materials modelling must consider data - either input parameters, or data for validation of the output. Any planned modelling activity must simultaneously consider data availability (and cost), as this constrains the likely success of the work as much as choosing the appropriate modelling technique and software. Some specialist modelling activities are very constrained because the experimental database is very sparse, and expensive to build up (e.g. high velocity impact experiments on new materials).

The selection of modelling technique in itself requires some consideration of the data requirements - data and software cannot be considered separately. A balanced view is needed: there is no point running expensive software

without the data to exploit it - and conversely there is little value in expensive data measurement programmes for which no computational use has been established. Whatever level of complexity and associated cost is chosen for data and software, the justification for it must ultimately be the value of the information required from the model by the end-user.

Consideration of data needs and how it is to be gathered is an important step in the construction of a model, as it is often time-consuming and costly. Its perceived importance depends on the background of the modellers. Model developers with a strong bias towards numerical analysis techniques typically play down this topic. In contrast, industrial practitioners place a greater emphasis on data gathering.

### **Boundary condition data**

Boundary condition data are as important as bulk property data. Two dominant boundary problems are:

- heat transfer coefficient (e.g. between cast metal or injected polymer and mould, or between dies or rolls in metal deformation processes)
- friction in forging, rolling, extrusion and machining

Two general modelling methods are now being applied to these types of contact problem:

- directly modelling the localised processes on a finer scale ("micro-FE")
- direct measurement from instrumented experiments, analysed by "inverse modelling" techniques

Inverse modelling means running a model backwards to infer what various "inputs" must have been to give the known "outputs". It offers a powerful approach to understanding complex boundary problems such as surface heat transfer, which can be very difficult to measure directly. The inverse approach is therefore to measure the distribution of the field variables (such as temperature) that are influenced by the boundary parameters, and then to solve the "inverse problem" to infer the boundary parameters. The technique has wider potential than interpreting boundary conditions, e.g. in sheet forming it is used to calculate the shapes of dies or metal blanks needed, given the shape of the component to be made. For further discussion, see Sargent et al. [1993] and Wood [1993b].

## **Models limited by data availability**

There are two major complications which mean that a valid research model of a process may exist but might be useless for industrial transfer because of a lack of data:

- there is no industrially-sensible method for obtaining the data (e.g. parameters that have to be measured from extensive transmission electron microscopy)
- the model predictions are very sensitive to minor variations between material compositions

The extent of the influence of changing composition in a given simulation depends on the underlying physics. No single code validated on one or two alloys can automatically be applied to a different alloy, even one which is superficially similar. Too many sweeping statements are made about what a piece of software can do, when there are fundamental yet subtle differences in the physics, the significance of which can only be judged by a reasonably well-informed metallurgist.

## **Initiatives in processing data measurement**

Modelling generates a continuous need for good experimental work: the support of modelling can be a fully justifiable basis for a lab-based project. Modelling throws up some of the most interesting challenges in materials research - matching this with lab-work is often even more demanding. Interaction is essential - models should guide experiment and vice-versa.

Data measurement to support scientific modelling activities is likely to be based in universities. Data gathering for industrial model implementation is conducted by individual companies, or by organisations such as the NPL (in collaboration with academia and industry).

The NPL is the lead organisation in the DTI-funded MMP programme for measurement of data for materials proposing. It was not immediately apparent that modelling had a central role in the co-ordination of the MMP programme. It is now clear that the situation has improved enormously as the principal players in the programme include model developers and users. This is certainly the case in MMP4 (thermomechanical behaviour during processing), and MMP2 (liquid metal processes) [NPL, 1996] but is probably the case across the programme. The balance of the programme aims for about 50/50 support for cast metals and metal working. Some consideration is also being given to transfer of metal working knowledge to machining processes.

There is a clear national need to assemble non-competitive data, but model users often say that data which was not measured in-house is rarely quite

what is wanted. Government-funded initiatives tend to concentrate on techniques for measurement, not assembly of databases. There is a role for trade associations here. Another mechanism is pooling data within a "club" of related industries. The NPL (and similar organisations) play a key role in addressing these issues of national data resources. There is a real need for data for processing, but measurement programmes have not always been very successful, or properly validated. Processing data is particularly difficult to document reliably, due to the close coupling of many different physical effects in any situation. A great deal of background information needs to be retained with any parameter values or else the information can be rendered worthless.

## **2.6 Scientific developments in materials modelling**

Academic research in materials modelling spans a wide spectrum, from the more applied materials engineering end, implementing existing knowledge into engineering problems, through to fundamental materials physics aiming to predict behaviour from an atomistic or other materials science perspective. The common thread throughout is material microstructure.

### **Modelling of material microstructure**

Many opportunities now exist to exploit the sophistication of FE output in describing processing or service conditions in great detail. Building in the capacity for prediction of microstructure into FE computations is a popular current theme. An important distinction should be drawn between microstructure prediction as a post-processing exercise (which is relatively straightforward), and having real-time microstructure-based constitutive behaviour, which potentially brings a huge computational penalty. It is very important to have established to what extent a reduced model of the constitutive behaviour is insufficient, before adding the complexity of real-time microstructure evolution. The additional complexity is liable to bring in many new assumptions and uncertainties in the data used for the microstructure model, so it is easy to create an illusion of progress. Cellular automata models offer a promising route for linking models of different types of physics at different size scales, since the CA model can run in parallel at its own appropriate time-step, updating the FE analysis when necessary rather than at every iteration. CA methods have only been extensively applied to solidification [Rappaz and Gandin, 1993], though preliminary work on recrystallisation is likely to go further [Davies, 1997].

The detailed output of FE and FD computations also now enables modelling to tackle the transient conditions of real processes, as compared to the idealised steady-state conditions. In thermal processing involving phase transformations, the importance of continuous cooling compared to isothermal conditions has long been recognised - at first empirically (e.g. CCT diagrams for steels) but increasingly in thermodynamic and kinetic modelling. In deformation processing this is less true, since most microstructural analyses consider only average temperature and strain-rate (often combined in the "Zener-Holloman parameter"). Experimental test data for hot forming is almost exclusively isothermal, constant strain-rate.

Greater predictive capability can now in principal be obtained by following the local thermal and deformation history (easily obtained from FE), since significant microstructural effects occur precisely because of the transient conditions. In general this is initially a matter of applying established physical metallurgy, in a more complex situation, but work of this type frequently poses demanding questions about the underlying physics. Differential state variable methods are very suitable for this work, as promoted by Ashby, Richmond and others [Ashby, 1992; Richmond, 1987, 1988; Bratland et al., 1997].

Predicting the effect of composition on microstructure evolution and properties is another popular current theme in materials modelling, which offers great potential for reducing empiricism. Recent examples in the Al industry, with alloy development for car body panels, or improved aerospace alloys for thick sections, show that such work is still largely empirical [Sainfort et al., 1996]. This implies extensive factorial experiments, mapping out processability or properties on 2D composition diagrams for a matrix of the dominant alloying elements. Physically-based modelling or artificial intelligence methods should now be able to make substantial inroads into the cost and timescale of this type of development.

Thermodynamic and phase transformation computations (including non-equilibrium conditions) for varying composition are very much more advanced in steels than other classes of alloy. Neural net methods have also been employed to link composition directly to properties, e.g. for toughness of steel welds [Bhadeshia et al., 1995; Ichikawa et al., 1996], and consideration is being given to other alloy systems and properties. A recent example quoted by the Foresight Materials Panel of a model-based derivation of a new composition was a rail steel which gave improved toughness without loss of wear or fatigue performance [OST, 1995b]. Similar opportunities exist in most metal alloys, and in polymers. Attempts to predict the effect of composition on processing behaviour and properties are closest to realisation for well-established materials and processes - inevitably a new process or material will take time to reach this stage for lack of data.

## **Linking length scales and multi-physics models**

The enormous growth in computer power has led to a surge of interest in addressing the physical complexity in material behaviour. As noted above, in many areas of processing or performance, continuum scale modelling (mostly by FE analysis) is very mature. The challenge to many modellers is how to build in detail from finer scales - two recurrent themes are therefore linking length scales, and multi-physics modelling.

Multi-physics modelling, or modelling a hierarchy of length-scale, open up an infinite variety of problems. It is always important that modelling is appropriate to the problem in hand, but this is especially so as the complexity increases. A useful output of such modelling should always be a clearer identification of the first-order gaps in scientific knowledge. Many comment that the potential for fully predictive models is often oversold, or that models are made over-complex only to predict things which can never be measured or which are of little practical interest.

This aspect of materials modelling has generated a lot of momentum in the UK, with the possibility of an EPSRC initiative dedicated to this topic. However only some of the research challenge in materials modelling is multi-physics or linking length-scales. To keep these activities in perspective, and not simply carried along by their own momentum, it would appear preferable for multi-physics modelling and length-scale modelling to be recognised within wider processing or performance initiatives, in which all modelling work can be assessed for its appropriateness for the problem in hand.

Multi-physics models require development in numerical methods to handle the solution of problems with many coupled boundary conditions. Micro-models are never actually plugged-in to a macro-model used for commercial work. An appropriate micro-model is used to generate a higher-level approximate description of the phenomena in the regime of interest, and this approximation is passed on to the model at the next higher level.

In some cases, what is perceived as the dominant limitation to macro-modelling generates activity in relevant micro-modelling. A good example is the current work on friction and heat transfer, where average values have long been acknowledged as inadequate, but obtaining better information requires a whole research programme of micro-modelling and experiment.

Multi-physics codes for materials processing create a huge demand for parallel computing, and will consume whatever computer resources are provided. As the complexity of such code goes up, it becomes more open to criticism: Has it been sufficiently validated? Couldn't the increased power be used for sensitivity analysis to sort out the first-order effects from the rest, and some "reduced modelling" conducted? How many industrial users can really benefit?

The appropriate length-scale or multi-physics connections to be made are specific to the class of material and type of behaviour being modelled. This is illustrated by noting a selection of current activities.

#### *Metal casting*

Multi-physics codes in metal casting are being developed to couple fluid flow, heat flow, and solidification with elastic-plastic deformation (shrinkage) [Bailey et al. 1995]. Macro-casting models are being linked to mesoscopic models for predicting porosity. To some extent the academic activity in casting is a long way ahead of the ability of industry to use it, though the need is greater for casting of structural components where integrity is more critical. Defect formation in casting is an area where the physics has not yet been captured sufficiently to give robust predictive capability.

#### *Metal forming*

There is a great deal of interest in linking length-scales in metal forming: to predict strain fields round inclusions or grain boundaries, shear localisation, or dislocation storage and subgrain structure (more as the controlling factors in recrystallisation than flow stress). The most fertile connections appear to be at this meso- to continuum scale (e.g. large arrays of dislocations, sub-grain to grain size modelling, as opposed to individual dislocation behaviour).

#### *Polymers*

Molecular-level simulation for development of new polymer compositions is now mature, having built on the success of drug simulation for pharmaceutical companies. There is now interest in developing a microstructural basis for predicting processing and performance, for structural polymers, filled polymers and liquid crystal polymers. This requires a move from the molecular to the microstructural (or meso) scale.

#### *Structural materials performance*

Linking intermediate length scales to continuum mechanics is also being explored for cyclic plasticity, crack tip behaviour in fracture and fatigue, grain-to-grain crystal plasticity and creep, and void nucleation in creep. This type of "micromechanics" is regarded by many as the most profitable scale to work on, with good potential for coupling to component level FE analysis, but it has so far attracted less activity than an atomistic or dislocation level view in idealised single crystals.

In fibre composites, the situation is rather different. A great deal of work has been conducted at the fibre-matrix level of detail for coupon size

behaviour. Continuum FE still has some way to go to exploit this knowledge, due to the nature of composite behaviour (anisotropy, matrix cracking etc). What is most lacking is meso-scale mechanics to transfer knowledge from lab-scale to prototype components.

### **Atomistic and molecular modelling**

The UK has several leading groups in atomistic and molecular modelling. Molecular calculations have made good headway in polymers and commercial software is growing rapidly. Atomistics research is generally fundamental in nature and remote from industrial problems. These methods appear more immediately promising for functional materials, rather than structural materials - e.g. impurities in electronic ceramics, semiconductors, nanomaterials etc. Modelling of polymorphism in organic molecular crystals and of optical and energetic functional materials is still at a fundamental science stage, but there is hope for greater collaboration with industry in these non-polymer areas.

In structural materials, the areas where this science is expected to first make a real impact industrially are in the behaviour of surfaces and interfaces. Examples are the modelling of dendrite tip solidification, phase boundaries in precipitation hardened alloys, oxidation, adhesion and wear, surface coatings, and the operation of catalytic convertors. Some large companies are keeping a "watching brief" or running feasibility studies, awaiting developments to be proven. Software (and suitably skilled users) in this area are very expensive - too great for a significant number of real industrial opportunities yet to emerge.

It is maintained that in due course atomistic techniques will mature for metals behaviour generally. Great care is needed in identifying the levels of microstructure which play a strong role between atom-scale and component-scale. The hierarchical complexity in metals is of a different character to polymers, and it is far from clear that the connections will eventually be made. It is clear however that there are many areas of metals processing and performance where there is little or nothing of industrial use to be gained from atom-scale computation until meso-macro connections have been understood to a much greater level of detail. Good demonstrator projects are needed in structural materials to show what is feasible using these techniques.

Atomistic and molecular modelling always demand parallel computing facilities. It is thus an area where hardware and software costs are significant, as well as the cost of well-qualified modellers to do the work. The lack of relevant data for this level of modelling in a wide range of materials can also be very limiting.

## 2.7 Industrial take-up

In the context of Technology Foresight a major issue is whether industry is able and willing to benefit from the materials modelling expertise and software available.

Models are much more computationally intensive than was the case only a few years ago. Most industrial modelling uses standard packages, often customised by the suppliers to a specific need. There is a definite shift away from writing FE code in-house, as commercial codes develop more features and user-definable routines. Modelling may also be contracted out to a specialised company. Some software suppliers may customise a package to a particular process for a client company, or act as supplier to a "club" of similar companies who share the costs and software provided. Confidentiality can present a problem however.

The major barriers to increasing use of models in industry are to do with how existing modelling technology is implemented, packaged and delivered. User-interfaces and pre- and post-processors have frequently been neglected compared to the computational engine in between, but there is an increasing awareness that the visible parts of the software are very important. The standard use of Windows for user-interfaces has contributed to a great improvement, and do-it-yourself packaging is getting steadily easier through software such as VisualBasic, or Object-oriented codes.

There are still strong cultural barriers to be overcome, even in industries which have had access to software for 20 years (e.g. polymer injection moulding). There are also many companies which do not use modelling, but it is not that they are unaware of its potential, rather that they have not got the resources to dedicate to it - particularly in sectors dominated by SMEs. Even where there is no cultural barrier to modelling within a company, it can be hard to keep people using models due to the commercial pressures on people's time. In any sector, there is a tactical issue as to how best to distribute software and provide the necessary education, training and support. National training centres have a significant role to play here.

It is also worth noting that modelling software for processing and design must take account of the steady increase in the number of standards and certification procedures which must be passed. This makes it essential that any code to be used industrially is properly validated and packaged in order to get ISO and BSI approval. For some new processes (e.g. laser processing) it has been commented that the existence of standards acts as an incentive to develop models, to help the emerging technology "catch up" with the requirements which are an accepted part of using a conventional competing process.

## Problems with Technology Transfer to Industry

The readiness with which modelling is practised in industry is strongly influenced by the level of technology to which the models are applied. "High" technology operations usually have more resources to set up experiments to provide data for the models, and have more expensively trained and experienced modellers. Deployment of the models either to production engineers or as part of a control system is not usually so much of a problem since both the process and the staff are already integrated with computer systems.

The ability of industry to absorb academic research and raise its value-added depends strongly on the market sector, and the size of company - e.g. easier in aerospace than in automotive, which is easier than construction. The advanced sectors and larger companies tend to attract funding as technology transfer is more straightforward. In terms of national impact however, there is enormous potential for wealth creation by relatively modest implementation of modelling in SMEs and lower technology production.

In many areas of process modelling, conversion of academic modelling expertise into usable software is lacking. There is a need for greater interaction between university and industry, and for mechanisms for producing acceptable software - either within universities, or intermediate research organisations could have a role here.

Industrial users will always have the following expectations of models: they should tell them what they know already by experience and empiricism, they must be quick, and they must be cheap. The reasons why the models produced by academics do not reach a production environment include (Sargent et al. [1993]):

- lack of support in writing user-interfaces - being of insufficient interest for academia, and too costly and time-consuming for companies themselves
- the results produced are not expressed in a way which the end-user finds helpful or even of interest (e.g. it has only been developed for idealised simple geometries and model materials, and can't handle real complex shapes and commercial materials)
- the physics of complex processes are not sufficiently developed to describe a wide range of conditions - the models are highly specific, so the potential market is small
- the demands for hardware, or data, or expertise in the user are beyond the viable budget in an industrial context - academic models suffer from a general neglect of considerations of economic viability
- models are perceived to replace creative people, rather than act as a tool for those people

There can be some inertia in adapting existing software in situations where a material substitution is being developed. In the same way that tooling for manufacture is largely dedicated to handling a given material class, so is the

software which has been tuned to the process. If modelling is an accepted part of tool and product design, modelling problems such as greater physical complexity or lack of data associated with the new material can significantly impede the take-up of the alternative material. Forming of aluminium instead of steel for car bodies is an example of this situation. Some regard this as the exception rather than the rule, i.e. many codes are to a large degree independent of material.

A more complex but important aspect of making software user-friendly and robust is the need for improved links between different stages in product analysis, from CAD to FE mesh to simulation to visualisation of the results. There are developments to provide direct links from CAD to thermal and stress analysis, within a single software environment, which greatly accelerates the product design cycle. Examples are the ELFINI Solver and Stress Analysis tools from CATIA (registered trademark of Dassault Systèmes, France) [IBM, 1996; Dreisbach, 1995]. There is also a growing need to feed forward the results of a simulation into subsequent analysis, e.g. the predicted gradient in microstructure or properties of a casting could be incorporated in subsequent stress analysis, or fed in as input to a heat treatment model. This is currently done in a laborious semi-manual way, but could become much more automatic, with significant potential for "product tracking".

### **Modelling entry costs**

In general, packaged software costs are much greater than hardware costs, and costs of software written in-house are greater still. Costs of personal computers or workstations have fallen so dramatically in recent years, that hardware is probably no longer perceived as a significant entry cost. At PC level, Matlab, MathCad, Excel, VisualBasic etc. are now much more powerful modelling tools, so writing code in Pascal, Fortran, C++ and so on is much less commonly required.

The true cost of modelling is dominated by manpower for programming and analysis, and the cost of acquiring materials parameter values (which can be very high if measured from a plant which would otherwise be producing product). Software costs are not entirely negligible of course, but it has been said by several people that the image of computer technology can be such that software purchases are readily authorised, even if it is never used in anger, while similar expenditure on unused machinery would cause an outcry.

## **Modelling centres**

Greater industrial use of modelling technology requires a ready point of contact for a commercial company wishing to model some practical processing problem. Conventional university research teams are not always appropriate for this role. Many academics are not in a position to be able to take broader issues into account and so develop modelling techniques which are inappropriate in an industrial context. The practical application of modelling technology would appear to be best done through shared research and development laboratories, trade association laboratories, national training centres, large consultancy companies or an equivalent of the German Fraunhofer Institutes or the 170 Japanese Kohsetsushi (public testing laboratories). In the UK, this role is increasingly being filled by "centres of excellence" within universities, in parallel with government and private laboratories.

A centre of excellence whose function is primarily technology transfer should ideally conduct modelling as one of a range of related activities (rather than only develop software), it should link modelling closely to real applications, and should exploit these parallels with other processes, crossing traditional boundaries. The commonality of much of the physical behaviour (e.g. heat transfer, material flow etc.) and software structure (e.g. CAD into FE) implies that there is great potential for technology transfer in modelling between widely different processes. Centres which work with disparate industrial sectors can exploit the overlaps which are often most apparent when the processes are viewed from a modeller's perspective.

A national modelling centre covering all aspects of materials modelling is not a popular idea. Organisationally it is preferable to embed modelling activity in a centre dedicated to a class of process. This may lose some of the potential for generalisation between apparently unrelated activities (e.g. die casting metals and injection moulding of polymers) but this is outweighed by the advantages of keeping the modellers closely in-touch with industrialists in that sector, and with in-house experimental research. An imaginative scheme might allow exchange of staff between centres, or a system of workshops, to enable cross-fertilisation of modelling approach between disparate sectors. This could require the setting up of a strategic group whose main purpose was to monitor progress in individual areas and to facilitate productive exchanges with other areas. A purely modelling centre would risk generating algorithm challenges instead of solving problems.

There is some distinction to be made between a centre which disseminates modelling expertise to industry in a consulting capacity, and a centre which aims to develop commercial code. There is now a global market for process modelling software. Code development to compete on this scale requires considerable organisation and an awareness of industrial needs. This is

beyond the capacity of most UK universities. It is the type of activity that might have been conducted extensively by Harwell or the CEGB prior to privatisation, and is regarded by some as an opportunity missed, when compared for example to French success in this area. Universities can only continue to develop code successfully provided sufficient commercial and software support is available. Some people propose that there is good potential for code development via user-groups, largely working together via the Internet.

## **Networking**

There is considerable support for better information about who does what in the modelling community in the UK, primarily to promote academic-industrial exchange, but also within academia.

It is becoming more common for the World Wide Web home pages of research groups to report on current work, and to include abstracts of recent publications, and for software to be released by this route. The Web is not uniformly regarded as an effective way to disseminate information within the UK. Its main role may be for international "science watch" activities. Information about activity in the US is easily found, while the UK and Europe lag well behind. However, a major problem with "self-publication" on the Web is maintaining quality. It has been commented that the international refereed literature is already of variable quality, but at least some screening has taken place. The Web is regarded as an unreliable source of information and data. In time it would seem likely that Journals will include Web information on authors.

From an industrial perspective, this route would currently only reach a small proportion of interested parties in any case, and may never be very effective due to the cost penalty in time spent using the Internet. An alternative electronic route would be to assemble information specifically on modelling on a free CD. This could be distributed (perhaps every few years) via the professional journals (backed up by hard copy for those without a suitable PC - it being expected that this will be very few in due course).

Broad discussion meetings such as the Materials Research Exchange in Birmingham (September 1996) are regarded by some as an inefficient means of bringing academia and industry together - it is a major time commitment for those participating, while the probability of getting real answers on the spot is very low. It is most likely that delegates go away armed with contact details, which in many cases could have been obtained electronically in the first place. However, the benefits of personal contact should not perhaps be underestimated, even if the contact serves only to pass enquiries on to colleagues. Some people fear that a modelling directory is simply

duplicative of the full research directories, so a more focused directory must be well set up and have a clear purpose.

The one-day meetings organised by EPSRC for its managed programmes are effective, as this provides direct contact with the relevant people. Consideration should be given to holding more one-day meetings in materials modelling. The breadth of the field requires careful consideration of the content, though imaginative modellers from surprisingly disparate areas can find plenty of ideas to exchange. Similarly considerable benefit can usually be obtained by bringing modellers together with the non-modelling experts (experimentalists or industrialists) with hands-on knowledge of the process or behaviour to be modelled (or controlled). Centres of excellence could play a leading role in this type of exchange.

It would be useful to be able to search for information on current research in a given field funded by EPSRC or other agencies. This is a laborious task using the published project summaries in an inter-disciplinary topic such as materials modelling. There are several networking tasks which could be eased by having a better referencing system on EPSRC funded projects (and those from other sources) - for industry seeking research collaborators or consultants, for links between universities, and for EU organisations interested in bringing in UK expertise. The addition of "keywords" to EPSRC grant proposal forms is to be welcomed as an immediate route to aid networking, national surveys etc. A more comprehensive picture of research can now be maintained than is provided by the rather ad-hoc, voluntary methods such as the Materials Research Exchange, BEST etc, but (very importantly) without placing an additional burden on those writing the proposals.

## **2.8 Education and training**

The educational demands of materials related degree courses in general was highlighted in the Technology Foresight document on Materials [OST, 1995b] and endorsed by the Aerospace Structural Materials Working Party [Institute of Materials, 1995]. Quite independently it was noted that materials modelling is a key development area. It might be added that the educational needs are particularly acute in carrying forward the target of increasing model development and use.

Materials modelling is a particularly demanding discipline, requiring a combination of materials science and engineering, numerical analysis and computer skills. The problem is compounded in the UK by the cultural problem that maths, physics, materials science and engineering are not

perceived as profitable career subjects by current students, in contrast to many other Western countries.

A closer integration of Materials Science with Engineering, Design and Computing is being steadily achieved. This particularly benefits modelling but is an essential shift in emphasis in many other ways too. While any number of curricula could be devised for Bachelors and Masters courses in Materials Science and Engineering, or as short courses for industry, the overwhelming message is that good modellers are marked out by *attitude* rather than technical skill. This is a difficult attribute to cultivate by teaching, but development of a questioning approach to modelling should be an underlying philosophy of such courses.

EPSRC potentially has a particular role in academic and industrial training for materials modelling. Consideration should be given to how this field could be supported within the EPSRC training initiatives (e.g. one week graduate schools, Engineering Doctorates, Research Masters, the Integrated Graduate Development Scheme, the Teaching Company Scheme, or Faraday Partnerships).

### **Materials modelling in university courses**

There has been a tendency for undergraduates on engineering or physical science degree courses to choose materials options if they are weak in numerical analytic ability. The numbers of school students choosing to study materials at UK universities has also been dropping for some time. Current courses are not producing either materials engineers or numerical analysis graduates capable of working effectively in multi-disciplinary modelling teams.

As computer literacy increases in schools and universities, it is possible that modelling could be exploited to make materials a more attractive option. Some universities are experimenting with using simple simulation software as a teaching tool. There is great potential for improved process visualisation, conveying the dynamic nature of processing in real-time, with opportunities to interrogate models for internal evolution of temperature, deformation, microstructure and so on. Coupling this approach with experiment is even more powerful. It is always important to convey that reality is not the model.

The need for a greater output of graduates with useful knowledge of materials modelling is uniformly supported, but is not easily achieved. It is not only a matter of teaching more modelling. Most materials science courses also contain too little on materials processing, or avoid the more complex variants (e.g. they cover continuous casting but not shaped casting, strip rolling but not forging). Modelling also implies an increased

requirement in teaching of computing - not just programming itself, but software engineering is also critical, with an increasing emphasis on computing in teams in universities. It has to be recognised that a higher modelling content in a materials course means that something else has to go, which can naturally meet with strong resistance. A second factor is that equipment and software costs to support the teaching of modelling are not negligible.

Post-graduate education in this area could take the form of one-year MSc courses, or modular training courses. There are some new courses or research opportunities in universities at Masters or Doctorate level which are aligned and supported by major industrial sectors - for example, research and training specialisation in ferrous metallurgy is now possible at a number of universities.

Materials modelling training however, should avoid too much specialisation. There is great potential for technology transfer in modelling between widely different processes which are not linked in most people's traditional classification of processes. This comes from the commonality of much of the physical behaviour (heat transfer, material flow etc). A second reason for breadth is to provide modellers with a good sense of what can be transferred from material to material. By definition, training for multi-physics and multiple length-scale modelling requires breadth.

It is implicit in all this that the expertise must exist within the academic staff of universities to provide the training. It was recognised however in the Technology Foresight report [OST, 1995a] that better training of the trainers in science, engineering and technology, with a high level of IT competence, should be given top priority. In materials modelling, these needs are particularly acute, since very few academics have the breadth of experience to teach modelling in any area than their own specific field, and may have little or no knowledge of the industrial perspective.

There may be a case for centres of excellence in materials modelling research also acting as centres for post-graduate training. It would be helpful if there were agreed criteria for what constitutes a good training in modelling, with some co-ordination and steering at a national level. This could best be achieved by bringing together academics from many areas of modelling problem and approach in several institutions, together with industrialists to convey the commercial context. The risk in leaving training to the free market is that individual universities simply tout for business, and sell "their" approach.

## Industrial perspective

Most industrial modelling groups believe there is no shortage of expertise in specific numerical and mathematical skills, but these are rarely coupled with adequate background in understanding the physical processes which cause the behaviour being modelled. It is also important to identify the different demands for model *developers* and model *users*. Opinions differ on the difficulty of recruiting qualified people for either modelling activity, but everyone agrees that more can be done to train people.

Industrialists express a strong preference for a mix of skills within a modelling group, but with breadth in outlook - an awareness of the strengths and weaknesses of FE and FD and analytical methods, an awareness of the materials behaviour to be captured, and a sense of the industrial context and economic constraints. There is no "ideal", as in different modelling sectors people express stronger preferences for particular skills - the only consensus is on attitude. Some people think the case is made too strongly for inter-disciplinary training, and that excellence in modelling or metallurgy is fine - provided these individuals are capable of functioning within a team.

Short courses for industry are required to bring industrialists up to speed on modelling methods and computer skills. Currently there are very few specialising in materials process modelling. It is not clear where such courses should be based, but as noted earlier, research centres may also take the lead as training centres in materials modelling. High quality modellers can come from a wide range of background: engineering, physics, chemical engineering, computing, mathematics, and materials science. It is often found that post-docs coming into materials modelling frequently make a significant change of field. The breadth of background therefore implies a variety of training needed to supply the academic and industrial demand for modellers.

The most serious manpower shortage is for people able to evaluate critically a range of possible modelling options and pick the most appropriate for the problem in hand. This requires the ability to perform the analytic modelling intelligently and to set up boundary conditions and materials models properly. The finite element method is often the default technique not because it is the best, but because the modeller is unable to pose or solve the problem analytically. Finite element models have the great advantage of producing a visual "result" within a defined period of time, whereas failure to derive an analytical solution means there is no result at all. The ease of producing impressive-looking coloured graphical results from a numerical simulation, even if they are actually of limited technical value, should not be underestimated.

There is real concern expressed that as the packaging of software gets better, but also deceptively "glossy", the dangers of people using software with insufficient knowledge increases. The proliferation in competing software as each industrial sector matures also requires greater powers of discrimination, either within companies or in the consultancies which they might approach for advice. Proper training, with a critical and imaginative attitude, are essential.

# Aspects of Materials Modelling in different material and process sectors

### Introduction

This section considers different material and process sectors individually. The information is based on the interviews conducted and the questionnaires received for this review, supplemented by views from two earlier reports for EPSRC on process modelling (Sargent et al.[1993]), and materials processing (Hollox [1993]). It is impossible to be exhaustive, but nonetheless it documents what has been said in relation to each of the areas covered. This serves to identify the real generic issues (assembled in section 2) and highlights the differences in approach, needs and maturity of modelling in the different sectors.

# 3.1 Casting

## Introduction

The foundry industry is based largely on aluminium-silicon alloys and cast iron. Large castings in titanium, steel, bronze etc. are a more specialised business, as are directionally solidified turbine blades, medical prostheses and investment cast jewellery. There has been a dramatic change in recent years in the casting industry, which now has a greatly improved image. This is partly helped by success with "high-tech" castings such as single crystal turbine blades, in which modelling has played a significant part. Casting modelling is dominated by shaped casting, with software now available at all levels of the casting industry. Many aspects of shaped casting modelling were discussed in the earlier review (Sargent et al.[1993]), and will not be repeated here.

This industrial sector in the UK is dominated by small companies, yet modelling efforts (like most research) are concentrated on the needs of the largest companies. Greater benefit to more of the industrial base of the economy would be generated by bringing the smaller companies up to speed rather than further extending the leading-edge activities of the larger companies.

## Shaped casting modelling

### *Uses of software*

Modelling of shaped casting now routinely covers:

- shape modelling and stereolithographic pattern prediction (really just geometric modelling)
- modelling shaped castings to improve "methoding" (mould and feeder design - placement of runners, risers, chills etc.)
- modelling of mould filling
- solidification, and macro-shrinkage

There is now no shortage of software for basic foundry needs - there are approaching 40 codes worldwide which do mould filling and solidification, and most do macro-shrinkage. These aspects of casting modelling are therefore saturated - the essential contents of the packages are much the same, while the only major differences are in the user-interface.

Consideration of the number of available codes is therefore important to avoid wasteful duplication.

The next demands made on software include the following:

- distortion and residual stress
- macro-porosity and other microstructural defects (such as inclusions, or lap formation)
- microstructure distribution
- stress analysis of castings

Only the bigger companies can afford to go on to these next problems. This implies a need for models which can describe the fluid to solid transformation in detail (including mushy zone behaviour), and the subsequent distribution of plasticity during cooling. Some rule-based microstructure and porosity prediction can be done, but the physics of micro-porosity is still not sufficiently understood to do much better.

Deeper physics modelling of dendrite growth or fluid flow through mushy zones does not come with much industrial push. The bigger the code the smaller the market - it becomes less clear who or what multi-physics codes are for from the industrial perspective, and they should be justified more as increasing scientific understanding, rather than as having a big commercial payoff.

There is an increasing use of simulations to design the casting itself - not just to design the mould system to make a specified part. Modelling also allows much larger single castings to be investigated than it would be economical to try empirically. Larger castings are attractive since they give a reduced parts counts (and cost) and fewer joining problems. It is interesting to note that high quality casting for aerospace applications has become more viable thanks to modelling - e.g. Airbus baggage door Al casting [Rendigs, 1996].

In-process monitoring and control in shaped casting appears relatively neglected. More can certainly be done, and usefully integrated with modelling.

#### *Industrial uptake*

Of the 750 foundries in the UK (almost all SMEs), there are reckoned to be about 50-60 using simulation. For comparison, in the Western World it is estimated that about 10% of the 9000 foundries have licences for casting software, of which 3 are dominant (MagmaSoft, Solstar and Procast). In Japan there are fewer codes, but about 35% of the 1000 foundries use them. The faster uptake in Japan partly reflects the fact that software for the Japanese foundry industry strategically aimed at PCs, using empirically-

based modelling. China has one main code, with currently relatively few users out of its 14,000 foundries.

When companies consider the costs of casting modelling, there is a tendency to consider the software only (somewhere in the £10k-100k range, though 3D CAD software may be needed as an add-on). The real cost is having properly trained people dedicated to using the software. Hardware is a minor issue - PC-based code is appropriate for SMEs, so the costs are negligible, while larger companies will readily support workstations.

It is commented that one weakness of the DTI CAST initiative was insufficient attention being paid to dissemination into industry. Many foundries do not use modelling, not because they are unaware of its potential, but because they have not got the people to dedicate to it.

### *Software engineering*

The modelling of shaped castings is dominated by one over-riding consideration: parts are made by casting *because* they are complex three-dimensional shapes, difficult to fabricate by other processes. Thus complexity of shape is fundamental. Modelling shaped castings is dominated by the need to predict the effects of different shapes for well-characterised alloys, not casting of new alloys. This implies that meshed methods are the major technique and that generating the mesh for complex 3D shapes is unavoidable.

Current commercial casting simulators are general tools for many different types of material and casting. Developing modular code which can be customised, sold-on and supported by specialist intermediaries across hundreds of process and alloy variants is a challenge primarily in software engineering, but this will have a major impact on the use of modelling by SMEs [Sargent et al. 1993].

The most demanding customers require validated modelling from their suppliers as part of their quality assurance. Large aerospace and automobile companies in fact now interact with their supplier foundries via modelling - CAD drawings supplied by the company are turned into a casting simulation which is sent back to the customers. This generates new software engineering demands: the links between CAD - FE mesh - simulation - visualisation of process all need to be more robust. The most time-consuming step here is converting from CAD to FE mesh - a step which will become progressively faster and more automated as integrated software develops.

There is also a growing need to feed forward the results of a casting simulation into subsequent analysis, e.g. the gradient in microstructure or properties of a casting can be incorporated in subsequent stress analysis, or

fed in as input to a heat treatment model. This is also currently done in a laborious semi-manual way, but could become much more automatic.

## **Modelling Centres**

As noted earlier, there has been steady growth in integration of modelling with foundry practice, and yet much more needs to be done relative to overseas. To facilitate the necessary technology transfer, there are now several semi-independent centres developing casting software and/or offering expertise, such as the Casting Design Centre (Sheffield), The Casting Centre (Birmingham University), and the groups at University College, Swansea and Greenwich University.

These centres have very different philosophies and emphasis, both in terms of their industrial interaction, and the type and complexity of software. The UK has groups working at every level from quick PC-based codes (largely rule-based) primarily for mould filling, to complex multi-physics codes which can only be run by the code developers themselves. The academic Centres prefer longer-term continuous relationships with companies (both supplier foundries and OEMs), rather than taking a trouble-shooting rôle.

Most groups offer expertise in a single code - but an exception is the Birmingham Casting Centre. This does not develop code, but develops use of existing codes with industry, and offers comparison of their relative benefits, also conducting a certain amount of benchmarking across 8 competing codes. The number of codes and the claims made about them is already becoming bewildering to the non-modelling foundryman, or to the model-literate designer with only a limited knowledge of casting, and the number of packages can be expected to increase. No one code is appropriate for all casting problems. Even large companies can't support more than one or two competing codes, while SME's may not even be able to afford to run one.

Consultancy of this sort is therefore of great value, as are other mechanisms for raising the modelling awareness of industrial customers to help them make the right decision on which models to use, or in some cases whether to use them at all. Software suppliers are naturally most interested in maximising sales. Not all software delivers what is claimed of it, or is properly validated. Validation also means different things depending on your point of view: e.g. some users may emphasise validation of predicted properties, while others are concerned with better process control during processing.

The experiences of the casting industry should serve as a warning in up-and-coming areas where there are currently relatively few codes, but which are rapidly reaching the maturity of the casting industry.

## **Other casting processes**

There is extensive modelling activity in liquid metal processing, but the details are beyond the scope of this review. Much of the purpose of modelling in this area is to save on energy costs and to maintain continuous high-rate production - e.g. in extraction (steel blast furnaces, electrolytic reduction of alumina) and in subsequent handling before casting (ladle temperatures etc).

Continuous casting processes are dominated by primary production of aluminium alloys and steels. Direct chill casting models for aluminium alloys are quite mature, including residual stress and microstructure prediction (details of some European work in this area were given by Sargent et al.[1993] - similar expertise exists in the UK). Work on steel is largely related to process modifications - e.g. control of ladle temperature, changing liquid metal flow into the concast mould, and control of bending rolls to avoid metallurgical problems.

Superheat temperature has a critical effect in continuous casting of steel, requiring modelling of the whole process including the temperature history of the ladle. This presents difficulties due to inadequate thermal property data for ladle refractories. The "experiments" are on an impressive scale, with instrumented ladles on operating plant. The effect on operator training of seeing models simulating their process is also considered very beneficial.

Modelling of the concast process itself is rapidly maturing, and approaching PC-based on-line code. The temperature history with complex heat transfer between strand and rolls or spray is now well-characterised, again by using full-scale instrumented plant.

The development of strip casting of steel and aluminium has been largely empirical so far, with commercial trials underway - modelling could play a greater role here.

Modelling occasionally fills an unusual role in being used to predict quantities of established importance which are difficult or impossible to observe experimentally (which naturally presents problems with model validation). An example of this in liquid metal processing is clean processing of steels, where impurity levels can be so low that they are difficult to detect in a statistically significant way. There is some work on improved measurement techniques for high purity melts in the new measurement for processability programme (MMP) at the NPL.

## Data

There are many data limitations for both routine implementation of current software, and for deeper physics modelling. Important but fairly routine measurement is needed for thermal properties and viscosity. Much more demanding are the needs for high temperature materials data near melting, and fluid flow and deformation behaviour of mushy zones.

Many data problems imply the need to develop more sensitive equipment and techniques. The new DTI-backed Materials Processability Programme on liquid metal processes is addressing these issues, and has clearly taken on board the importance of modelling in this sector [NPL, 1996]. It is essential that data collection and development of measurement techniques are co-ordinated nationally, and that data experts communicate with modellers to ensure a supply of appropriate information for simulation work.

Different alloys offer greater and lesser problems in a given simulation depending on the nature of the underlying physics, for example, nucleation behaviour is strongly alloy-dependent. Code validated on one or two alloys cannot automatically be applied to a different class of alloy. Too many sweeping statements are made about what a piece of software can do, when there are fundamental yet subtle differences in the physics, the significance of which only a reasonably well-informed metallurgist can judge. Sargent et al. [1993] point out that, because of the lack of data or understanding of specific phenomena for particular alloys, the foundry engineer has to use models knowing *how* they are inappropriate and *where* their results will be misleading.

## Underlying materials science

There are many materials science/engineering challenges to be solved in order to enable casting simulations to include physically-based predictions of, for example, microstructure, porosity, residual stress, and cracking. Particular issues are:

- conditions at the mould-metal interface
- fluid flow through mushy zones, and deformation of solid-liquid structures
- sintering of refractory moulds
- incorporating microstructure models into macro-FE models (e.g. using cellular automata methods)
- thermodynamics and kinetics of alloy phase transformations

Alloys vary enormously in the number, morphology and complexity of phases which can form during solidification, or in the solid-state during cooling. There has been a resurgence in thermodynamics in response to this:

e.g. phase field modelling, or linking of dendrite growth to the thermal field  
- rather more than prediction of the phase diagram.

Further advances in casting modelling are potentially very multi-physics. Multi-physics codes are being developed which couple fluid flow, heat flow, and solidification with elastic-plastic deformation (shrinkage) [Bailey et al 1995]. Mesoscopic models for predicting porosity from the macro computation are under investigation. This work creates a huge demand for parallel computing, and should be regarded as one end of the spectrum, rather than the norm. It should not be assumed that the only advances to be made are those which link all possible physics - from the commercial point of view it is most important to identify and solve the first-order problems.

## 3.2 Thermomechanical Processing of Metals

### Introduction

This section covers a wide range of processes: flat-product and shaped-section rolling, forging, extrusion, sheet pressing and drawing. Heat treatment is a closely related topic, so a few remarks are also made here.

For many years there has been a lot of effort on forming new materials, such as MMCs or intermetallics, at the expense of conventional structural metals. This situation is changing - thermomechanical processing of traditional materials is a resurgent research area, with strong university centres in Sheffield, Swansea, Birmingham, Bath, Cambridge (and others), and a Managed Programme starting in EPSRC.

A major recent development is the launch of a new centre in Sheffield ("IMMPETUS"). The focus of the centre will be rolling of flat products and section rolling, with closely integrated modelling and experimental activities. It offers an almost unique blend of metallurgy, thermomechanical analysis and control engineering, combined with close links to industry.

The forging industry is in many ways reminiscent of the shaped casting industry, prior to the casting initiatives. The national programme in forging (Forging 2000) is timely - modelling should be a key element here, with the goals of improving design of both tooling and components, giving better shape and property control, and predicting microstructure and properties in a wide range of materials. The parallels with casting should be exploited, and lessons learned from past experience:

- identifying the appropriate levels of model complexity and software to develop
- developing code which is flexible, and easily tailored to a wide range of products, materials and problems
- identifying data and measurement needs
- planning how to disseminate modelling software and expertise, to the benefit of both large companies and SMEs

Forging, extrusion and sheet pressing are processes where modelling is potentially particularly powerful as production involves a huge range of shapes (often thousands per year), and the shapes are inherently 3D (extrusions may be prismatic, but the dies and metal flow through them are 3-dimensional). For these processes the costs of tooling and dies are

particularly high, giving clear benefits of modelling for designing both component and tooling. Extrusion modelling is a large-scale activity abroad, but has lost some backing in the UK since Alcan withdrew from the extrusion business.

Much of the research and modelling in thermomechanical processing is also relevant to related “hot deformation” processes, such as machining, friction welding etc. Machining in particular is an area of huge economic importance, which does not attract research activity in proportion. It was pointed out by Hollox [1993] that tool technology in general (cutting tools, forging and extrusions dies etc.) is a critical but relatively neglected area for research.

## **Modelling status**

### *Industrial setting*

A great amount of industrial modelling is performed on thermomechanical processes. Continuum mechanics FE is well-established, both for simulating the manufacturing process itself and also the less obvious task of modelling the standard tests used, for example, to determine constitutive behaviour. There is a unanimous view that the greatest limiting factor in all metal forming analysis is poor characterisation of interfacial friction conditions, and to a lesser degree heat transfer.

The more complex the geometry (or the less constrained the deformation), the greater the difficulty of the FE implementation and the scale of computation demanded. FE codes cope well with modelling the simpler geometries like flat product rolling, and are used routinely by both metal and equipment manufacturers, for control of flatness, shape and so on. For section rolling, forging or extrusion the inherent 3D flow behaviour is still frequently limited by computational power. In rolling and extrusion, a further problem is the distinction between steady-state deformation and the initial and final transients, which are much less well-characterised. Forging is almost continuously transient in nature.

The complexities of anisotropic yield behaviour tend to be important only in selected areas, notably sheet pressing. The complexity of model needed then depends strongly on the type of alloy, e.g. how well the material formability can be captured by “forming limit diagrams”. This approach and the common yield criteria are much less valid for most aluminium alloys than for steels, and there are similar problems in titanium alloys (including superplastic behaviour). Cold formability of a range of aluminium alloys is a research activity receiving a major push from the development of aluminium in cars.

Incorporation of anisotropy and texture into sheet forming modelling is a further problem which is still limited by affordable computer power, and is therefore only accessible to the large aerospace or automotive companies. The justification for this type of modelling again comes from the very high cost of trials (particularly in aerospace).

Benchmarking of different codes has been practised for many years in sheet stamping - e.g. comparing predictions for standard sheet stamping tests. It has been much less so for bulk metal-forming, but should be built into any new initiatives in (for example) forging. Standardising codes is not desirable however in the same way that empirical testing must be - the key element is flexibility, so that a single code can be matched to a diverse range of problems, and a range of codes is available for a given problem since no one code can handle all problems at the appropriate level of complexity.

It is important to consider the hierarchy of suppliers in a given sector. The major suppliers to large automotive or aerospace companies are not now small companies. The character of many SMEs has shifted to being single-product suppliers to much larger suppliers higher up the hierarchy. This should be taken into account in any initiative which purports to develop technology for SMEs. The supplier companies able to exploit modelling, for example, may no longer be SMEs at all. There are also distinct differences between casting and metal forming. In net-shape processes like casting there is a clearer link between design and process with in consequence a clearer case for using software; metal forming SMEs are generally further down the supply chain, so it is harder to identify the modelling need. Machining is even more remote from the design process, so modelling of machining has a very poorly-defined role.

#### *Modelling needs in metal forming*

The main areas of fundamental research needed in metal forming are:

- interface conditions (friction and heat transfer)
- microstructure evolution and coupling to FE
- understanding of deformation in inhomogeneous materials
- robust software engineering to facilitate information transfer between CAD, FE and stress analysis (as discussed under shaped casting, but equally pertinent here)

In the first three, a combined approach of numerical modelling and experiment is essential. FE methods are being developed to tackle some of the micro and meso-scale modelling itself (e.g. crystal plasticity codes, micro-FE of friction at interfaces). From an industrial perspective, the need for improved understanding and modelling of friction and heat transfer for continuum FEA continue to dominate. This forms a major part of the new NPL programme in measurements for materials processing (project MMP4),

which includes development of new techniques for measurement. Micro-sensors may be of great value here.

### *Microstructural modelling*

The view has been put forward that FEA has far outstripped the physical metallurgy which can be done - either to refine the input constitutive behaviour, or to predict structure and properties using the FE output. The level of this perception differs quite strongly between the main metal classes: steels, Al alloys, Ni alloys, or Ti alloys. This to an extent reflects differences in underlying metallurgy and also the complexity of shape being formed (e.g. flat products with difficult texture control in aluminium, section rolling with distortion and residual stress critical in steel).

Formed metal products are almost all sold on the basis of the quality of their shape, residual stress levels, and properties. The need to specify microstructural details (distribution as well as average) is steadily increasing. At present the commonest specification would be for grain size and texture information.

The established empirical approach in hot working has essentially bypassed microstructure, by using the Zener-Holloman parameter (which combines strain-rate and temperature) and the von Mises equivalent strain to predict flow stress and recrystallisation behaviour. This has worked well for some steels and is used industrially, but has been found to be much less applicable for other materials, and not sufficient for modelling damage in forging of any materials. There is growing interest and research activity in building more detailed understanding of microstructure evolution in hot working, including experimental work (strain-path effects for example), neural net analysis, and state variable modelling.

There is a great deal of interest in linking microstructural length-scales in metal forming. The most fertile connections appear to be at the meso- to continuum scale: e.g. strain fields round inclusions or grain boundaries, shear localisation and fracture (failure during processing), dislocation storage and subgrain structure (more as the controlling factors in recrystallisation than flow stress). New experimental techniques are giving a great boost to the viability of this type of modelling activity (EBSP, automated TEM for microtexture etc). Atomistics does not appear to have a direct role in bulk deformation modelling, except perhaps at a very fundamental science level in, for example, dislocation solute interactions.

Research at this level is very relevant to tracking microstructure through multi-stage processing, e.g. how the as-cast structure influences the effects of forming, or how the as-deformed structure influences the effect of subsequent heat treatment or welding.

A recommended approach to modelling of microstructure is the use of differential laws for evolution of internal state variables. This route has the advantage of being able to follow the transient processing conditions which are the norm in industry, and the ability to capture the continuous evolution of structure in multi-stage processing. Most microstructure evolution laws in materials science have been formulated for isothermal conditions, and at constant strain-rate for a deformation process. The generalisation of these laws to transient conditions is a matter of current research. Work is also being conducted on training neural nets with experimental data for microstructure combined with the process history computed by FE analysis.

Microstructure prediction as a post-processing exercise following FE computation is now largely feasible, using the element-by-element temperature, strain, strain-rate histories, though actual case studies are few. This is a big advance in capability, which was previously limited to the behaviour predicted by average conditions, often only on the product centre-line. However, even simple microstructural models only tend to be validated and used for selected material grades and products in industry.

Fully integrating microstructure-based constitutive laws into FE comes at a large computational penalty, with increased uncertainty due to the data used to calibrate the microstructure model. The cellular automata approach has yet to be explored in any detail for coupling structure evolution and continuum FE analysis in forming processes. It is important to ask whether the perceived benefit of the complexity is going to be detectable, particularly in view of the first-order problems associated with friction and heat transfer. This level of activity is at present therefore confined to research models of hot working.

It is a stated target of Foresight to link composition to processing conditions and properties. Making such connections in thermomechanical processing can introduce very major complexities, the degree of which is also very dependent on alloy class. The Foresight recommendation is perhaps a bit sweeping - these complexities should be recognised, and appropriate targets set for modelling (and measuring) the effect of composition. In Al packaging alloys for example, idealised alloys (Al+Mg, or Al+Mn) can be handled quite well, while commercial canning alloys (Al+Mg,Mn,Fe,Si) are still a long way down the road. Ni alloys are rather more forgiving than Ti alloys, steels are more forgiving than Al alloys, and so on.

## Heat treatment

Thermal modelling is largely mature for problems such as furnace design, bulk heat treatment of coils and so on. In contrast, component heat treatment (particularly quenching) is still largely a “black art”, with very little research activity supported by EPSRC (or other agencies), yet all metals are heat-treated in some way. Internationally the importance of the subject is recognised - it was the subject of a whole US conference in 1997. From the modelling perspective, inverse modelling techniques have been shown to be very powerful to infer complex surface heat transfer conditions, from data collected at positions in the bulk.

Thermal analysis serves two major purposes - as input to predicting residual stresses, and for predicting microstructure and property evolution. Residual stress prediction (mostly for metals, but also now for polymers) is usually to minimise problems, though there are also examples where deliberate controlled residual stress is used to enhance performance (especially in surface treatments).

For microstructure prediction there is great potential, as discussed for thermomechanical processing generally. Microstructure modelling for heat treatment is also usually directly applicable to welding processes, which effectively generates a transient thermal cycle. In both contexts, there is relatively little modelling work as both areas traditionally rely on empiricism. Modelling work is much more advanced in steels than other classes of alloy, but includes thermodynamic and phase transformation computations (e.g. CCT diagrams), and increasing use of neural nets to capture the combined effects of process and composition.

Carbon steels present particular challenges when modelling of the  $\gamma$  -  $\alpha$  phase transformation is coupled to deformation - for example during cooling of rolled plate. This is because the creep properties change markedly with this transformation, so the resultant residual stress and distortion is sensitive to temperature in a complex way. This is an unusual situation where the microstructure evolution is not an output of the exercise, but is a critical internal feature in determining the constitutive behaviour. The output is the residual stress distribution which is fed forward to a continuum mechanics analysis of the levelling and straightening operations.

## **3.3 Joining, Surface Engineering, Laser Processing, Ceramics and Powder Processing**

### **Introduction**

The topics of this section receive much less attention in research than any of the other sectors discussed in this report. As a result, modelling in these sectors is also relatively neglected in the UK. The industrial importance of joining technology, and increasingly surface engineering, cannot be underestimated - both were noted by the Materials Foresight Panel (OST [1995b]) and were strongly emphasised in the EPSRC's assessment of processing (Hollox [1993]). Laser processing, ceramic and powder processing are more specialised activities, but merit some comments on modelling.

### **Joining**

In joining technology in the UK, empirical methods have dominated development and form the basis of most processing and design codes. Software has mostly been produced as a more efficient means to document processing procedures (covering a wide variety of geometries, materials, and process conditions) or as a guide to weld performance. Hollox [1993] noted that joining is always left too late in material or product development, and recommended that greater attention be paid to joining within design and concurrent engineering. For models to be used in an industrial context, they would have to be a demonstrable improvement on the accepted existing design codes, databases or expert systems.

The UK's leading institution in joining technology is TWI (the former Welding Institute), but here the emphasis is on process development and industrial trouble-shooting. Development of new processes, or the increased use of existing processes on different materials, includes adhesive joints, diffusion bonding, laser processing, and friction welding (particularly the friction stir process). Modelling however has a very low profile in this work at TWI, but is supported by various academic groups.

Modelling of welding (especially arc welding) is an established field internationally, with a recent number of texts (Grong[1995]; Cerjak et al.[1992, 1994, 1996]) and a new journal launched in 1997. The potential of weld process modelling does not appear to be as well recognised in the UK as it is

in other countries. Modelling software is dominated by performance of steel welds. Most effort is concentrated on predicting residual stresses and distortion, which can usually be done with a fairly approximate treatment of the heat source, or on predicting weld performance (particularly fracture and fatigue). Welding design codes can be very conservative, e.g. taking the minimum strength of a welded joint as the design stress throughout a structure, or assuming residual stresses are close to the yield stress. Modelling may prove a means to develop less conservative codes, e.g. by predicting actual post-weld properties, or residual stress profiles.

Modelling of welding processes themselves is often very complex, and perceived by some to be too intractable (or costly). The number of alloy and process variants is huge, while the problems to be addressed range from optimising process conditions for maximum productivity, to controlling residual stress, distortion, and properties in and around the joint. It is precisely this complexity which means that modelling can make a contribution:

- to reduce the extent of experimental work required, and thereby to minimise cost of developing new processes or certifying existing procedures
- to provide predictions of operating conditions and final microstructure and properties - for designers, for use on-line, and for failure analysis
- to provide physical insight into the complex mechanisms involved in joining processes, leading to improved process control

Welding modelling can be conducted at many levels of complexity, from simple heat flow and microstructure models to “map” viable operating parameters, to detailed multi-physics models applied to individual joints. As always, selection of the appropriate level of complexity is an important issue, along with consideration of data needs.

Heat flow in welding may be considered by analytical or numerical (FD/FE) methods, depending on the job in hand. For modelling distortion and residual stress, numerical methods are necessary to capture the details of the joint geometry, and coupling the thermal history to deformation. Approximate geometries often suffice in modelling microstructure evolution, or developing new processes, in which case analytical methods are a good starting point.

Microstructure modelling is particularly challenging in welding, since the thermal history is entirely transient. Modelling the phase changes over a wide range of heating and cooling rates pushes established physical metallurgical modelling to the limit. Relating microstructure to properties is difficult - particularly for the toughness problems associated with welding of steels. For this reason, neural net methods have been explored as a pragmatic route to capturing the complexity (Bhadheshia et al., 1995; Ichikawa et al., 1996).

Welding offers a very good example of the potential for exploiting modelling to make connections in multi-stage processing. For example, little attention has yet been paid to the scope for modifying prior thermomechanical processing and heat treatment in order to enhance weldability. Similarly, modelling the effect of composition (in both parent alloy and filler metals) could lead to improved weldability without loss of other qualities. Such developments are inevitably very slow and costly by empirical means.

Welding has traditionally been dominated by steels. However, welding modelling is part of recent activity in superalloys (in one of the successful Foresight Challenge projects), and is now an important growth area in aluminium (especially for automotive use, but also for maritime and aerospace). In the automotive and aerospace sectors joining is an emerging area of activity, as both adhesives and welding take on a higher profile. A quite different joining activity in which modelling has been well-established for many years is reflow soldering for the electronics industry.

In adhesive joints, continuum and micromechanics approaches to predicting failure mode and loads receive some attention. The key need is for models which can describe the behaviour of real component joints under complex loading - not just lab-based coupon tests. Full component tests are expensive, so reductions in the number of tests give major cost savings. This exactly parallels the needs in composite structures. The effect of environment on joint integrity is critical, but the underlying behaviour of adhesive materials within loaded joints is often not yet sufficiently understood experimentally for much to be achieved by modelling.

## **Surface Engineering**

There are many parallels between joining technology and surface engineering. It is a relatively neglected area in research with great potential, and most research is empirically based. Surface treatments are also insufficiently integrated into the design process (Hollox [1993]).

As with many manufacturing processes, it is often stated that the emphasis in surface treatments should be on incremental improvement and increased uptake of existing methods (e.g. PVD/CVD, laser processes, and plasma/ion nitriding), rather than developing completely new processes. There has been a tendency to keep trying new coating materials empirically, instead of properly understanding the existing commercial materials (largely TiN based). In structural materials there has been a shift in emphasis in recent years from new materials research to improved processing and understanding of existing materials - it may be expected that surface materials will follow suit.

Activity in surface engineering covers a wide variety of materials, increasingly including polymers (e.g. scratch-resistant spectacles), and glasses (TiN coated windows), as well as steels, superalloys and so on. Modelling has roles in improving knowledge of the underlying science of adhesion, predicting mechanical performance, and in improved process control.

The dominant activity is hard coatings for cutting tools, based on TiN (also with C or Al), mostly using PVD or CVD processes. The inaccessibility of the component during processing makes this an intractable modelling problem - on-line measurements are difficult, but the process physics can be sensitive to local processing conditions at the surface, which may be rather different to the macroscopic conditions. Data for these processes and materials therefore tends to be sparse and unreliable. Modelling is currently limited to residual stress, and continuum analysis of the mechanics and failure mechanisms of coated materials in sliding contact.

### **Laser processing**

Laser technology is often regarded as a processing sector in its own right, but is closely associated with joining and surface treatment (as well as cutting). The UK effort is concentrated in the Laser Centre (TWI/Culham Laboratory) and a number of university groups. There have been some national programmes for developing laser technology, or increasing its uptake in the UK (for example the DTI "Make it with Lasers" Programme), but it is not clear why laser processing has been so much more successful in Europe and elsewhere than in the UK. Modelling of laser processing has been dominated by the underlying physics, rather than the application - this was discussed in some detail by Sargent et al. (1993). The potential for greater industrially relevant modelling still exists in laser processing - as with most joining and surface engineering processes.

### **Ceramics and Powder Processing**

Ceramics and powder processing include a wide number of relatively niche materials and processes. The commonly held view is that engineering ceramics have a very limited role in structural applications, but are far more important as functional materials (e.g. electronics, magnetic devices, superconductivity, fuel cells). Modelling of ceramic processing and failure is therefore most likely to have the biggest payoff here. The Foresight Materials Panel concluded that there was no evidence for more work on monolithic ceramics for dynamically stressed applications. The established niche markets for structural ceramics include cutting tools and armour.

This emphasis in applications of ceramics means that process modelling dominates. Modelling of mechanical performance is in any case difficult, since performance is dominated by toughness, which is a much harder mechanics problem than deformation at the continuum or microstructural level.

Densification modelling is quite well-established for sintering and HIPing, with models for density evolution as a function of particle size, temperature, pressure and time. Modelling can be used:

- to improve shape control
- to predict (and thereby avoid) grain growth
- to predict the grading of initial powder before compaction, which is used to improve density distribution

Powder compaction has been modelled as a materials science problem in diffusion and creep for simple stress states, and as a continuum mechanics problem to include general 3D stress states. Compaction models are very material-dependent, requiring calibration to extensive experiments, so tend to be largely research models at the detailed level. As the demand is much less than in the metals and polymer industries, very little progress has been made in linking material composition and process conditions to properties (though the physical coupling is equally applicable to these materials). Some limited modelling has also been applied to problems of microwave processing, and flow of powders or suspensions.

Hollox (1993) drew attention to related materials processing sectors, which have yet to reach their full potential, or are neglected research areas: powder metallurgy, refractories (for casting), chinaware, cement, concrete and other building and road materials. The traditional ceramic industries have a very low technology image, often having very high energy bills and large scrap rates. A greater scientific input could therefore make a significant impact, but this does not appear to have been emphasised by the relevant Foresight Panels. Modelling work developed for advanced ceramics or other porous materials (e.g. powder flow, densification and microstructure-property characterisation) could be applied fruitfully in all these areas, and merits further consideration.

## 3.4 Polymers and Composites

### Modelling status: polymers

Commercial polymer modelling falls into two broad categories: (i) modelling the major processes such as injection moulding, to support part and tooling design for improved processability, and to predict product quality (e.g. shrinkage, porosity) and properties (e.g. molecular orientation, elastic modulus); (ii) molecular-level simulation for development of new polymer compositions. Molecular-level software has built on the success of drug simulation for pharmaceutical companies. Biosym/Molecular Simulations Inc (based in California and Cambridge, UK) which covers both fields is now the largest materials modelling software house in the world.

The British Polymer Training Association is an example of a national Centre dedicated to improving the skills base for a particular industrial sector. While mould-fill software has been available for 20 years (longer than most metal casting codes for example), it is still not accepted by the great majority of companies. The Centre gives strong emphasis to processing simulation software in its training. An example is PICAT, a software system for improving injection moulding. The Centre argues that great benefit could be rapidly gained in the UK plastic processing industry if companies in this sector (predominantly SMEs) were all aware of and could make effective use of currently available software.

The mechanical response of polymers has traditionally been described phenomenologically. Further development here could be beneficial, for example to give more complex descriptions of relaxation or extensional effects on flow. There is greater interest in developing a microstructural basis for predicting processing and performance, as polymers develop for more structural applications, so that processing can be coupled to component properties. An example is performance of HDPE gas pipes, where attempts are being made to build in residual stress and crystallinity gradients inherited from processing. There is considerable scope for making connections through multi-stage processing, as in metals - e.g. from powder preparation through moulding to welding, and then service.

Industrial modelling is dominated by processing (e.g. injection moulding), though some consider the reliability of codes could be improved with greater attention to verification of the output. Academic modelling covers both performance and processing, and increasingly the links between the

two. Several research groups are now moving from the molecular to the microstructural (or “meso”) scale, with the ultimate goal of making connections at the continuum FE level. The driving force for this appears to be coming from the scientists rather than the FE community.

Most meso-scale work is applied to structural polymers, but increasingly also to composites, especially filled polymers. Related approaches are applied to modelling liquid crystal polymers, so in polymers the distinction between structural and functional is rather blurred. Elastomeric materials appear to be relatively neglected in comparison to the other classes of polymers. Performance can include some important polymer-specific environmental effects, such as photo-oxidation and weathering, for which both models and data require development. There is a similar challenge as in metals to link composition to processability and performance, via microstructure. Composition in polymers includes additives and stabilisers, which can cause problems as details may be proprietary.

Fundamental polymer science modelling includes phase transformations, polymer crystallisation, complex flow behaviour (such as the effects of chain branching, and distribution of molecular weight), and phase separation in the fluid state. The fundamental molecular understanding of the connections between microstructure and the macroscopic visco-elastic properties is still poor. Most developments have been for idealised lab conditions and clean model systems, but are now being applied in the more complex conditions found in real processes. This brings with it the attendant problems with data needs for input and validation, with more complex geometries and boundary conditions (such as heat transfer). This may call for semi-empirical modelling to fill in the poorly-characterised behaviour. The desire to link processing to product performance also introduces software issues associated with information transfer between the two. This requires a greater level of dialogue between the FE and the microstructural modellers.

These are very similar issues to those found in modelling processing of metals. Greater cross-fertilisation could therefore be beneficial: the metals casting and polymer moulding communities have a lot of challenges in common. How much communication is there between them? Traditional materials education would encourage very little - training materials modellers must encourage this way of thinking.

## **Modelling status: composites**

In composites, there is a continuous possible variation of “materials” to be considered, with the added complexities of layup and different fibre/matrix systems. This implies an infinite number of combinations - as with metal or polymer compositions - so models can be used to explore laminates prior to experimental work. Experimental prototyping of composite components can be very time-consuming and costly, so the returns in reduced testing and faster development are just as significant as in metals processing.

Composite modelling tends to be based in academia, with scope for closer collaboration with industry - though in this field it appears less clear how modelling can help solve the industrial problems. The current industrial emphasis (particularly in civil aerospace) is for low-cost manufacturing routes (such as resin transfer moulding). Modelling may have a useful rather than critical role here - e.g. there may be scope for thermal analysis and predicting distortion, or modelling of resin flow at low pressure. Other industrial needs include forming limits for deformation processing of discontinuous fibre-reinforced systems, for which modelling or data are very scarce. The dominant costs for aerospace developments in composites are associated with getting composite designs qualified. Modelling can contribute here, including modelling of impact damage (for which data gathering is particularly expensive).

Composite modelling has been dominated by performance, and there has been a long history of research in laminate micromechanics in the UK. This can be used to screen out problems at coupon level before moving up to prototype components, but there is a need to transfer lab knowledge to design of composite structures and to embed the knowledge in FE codes. It is increasingly possible to build composite models which take account of different lay-ups, with a wide variety of fibre/matrix systems, and including the effect of damage on properties. Such computations must remain within the scope of PCs or workstations to be of interest to industry. There is a need for "meso-scale modelling" in composites, which captures the essential effects of damage on properties. Direct linking of processing to performance is a very remote prospect for long-fibre composites - it is much more tractable for discontinuous-reinforced materials, where melt flow controls fibre alignment and thus properties.

As in other areas, there are difficult challenges in providing solid experimental data for input and validation of modelling. In spite of many years of academic research on failure mechanisms in composites, the failure behaviour of composites in real components (including the complexities of joints) has not been modelled satisfactorily.

In common with much work on metals, there is a danger in composites of software generating far more output than designers know what to do with - either in predicting laminate properties, or in FEA of composite performance. In this field, modelling software may well be the means by which the designers are instructed in how to design with composites at all, so the normal demands for good user-interfaces are particularly important.

Some aspects of composite performance require analysis beyond the scope of current software, so application of FE codes (or hydrocodes for high velocity impact) can require significant development of the tool in order to handle the particular constitutive response of composites, as the codes were invariably developed first for metals.



# Conclusions and Recommendations

### Summary

Materials modelling was given a high profile by the Materials Panel in Technology Foresight, and the survey fully endorses this view. Materials modelling is a very diverse topic which impinges on many Foresight sectors. This survey has not attempted to review the whole field but has focused on "structural materials" in processing and service. Other important industrial sectors should be considered in some depth: extractive processing, surface engineering, building materials, refractories for casting, ceramics for electronics, semiconductor and other functional materials, and also sectors such as food processing. It is believed that many of the issues in these sectors will prove to be very similar to those discussed in this report.

The key development areas highlighted by the Panel, in which modelling has a role, appear to be generally well-chosen. The Foresight recommendations come however with the limitations of any "broad-brush" coverage: (i) the list of sectors or problems is not exhaustive, so important areas not mentioned explicitly could be placed at a disadvantage; (ii) broad statements about modelling needs can be interpreted too generally, when in fact their relevance is largely dependent on the process or material behaviour to be modelled.

## **Critical aspects of modelling**

Research in materials modelling requires three essential components: mathematical methods, materials science and computer/software science. This is still not sufficiently recognised in many research proposals.

There is a hierarchy of complexity in almost all materials modelling, whether for processing, performance or describing underlying physical behaviour. Choosing the appropriate level of complexity is an essential element of model building and use, and should exploit both approximate analytical and numerical meshed methods in selecting the appropriate software implementation.

Increased computer power is absorbed far too readily in added complexity, rather than in more thorough interrogation and sensitivity analysis of an existing model.

The data needs of a modelling activity, both for input and to validate the output, should be considered (and costed) from the very start.

## **Industrial process modelling**

The industrial takeup of process modelling is very non-uniform across different materials processing sectors. Traditional industries often lag behind in using process modelling.

Modelling of shaped casting is mature in terms of software tools for most routine industrial needs. A significant change of image has been achieved in the foundry industry in recent years, but the sector still has a long way to go in terms of adopting process modelling. Forging lags behind casting, and could benefit from a similar initiative in developing and implementing appropriate software tools. The large metal producing companies and equipment suppliers routinely use software for continuous casting and rolling processes. Modelling is part of making the case to win business in certain high performance sectors, and this can be expected to steadily expand as a requirement for suppliers of castings, forgings etc.

In current commercial code the emphasis is on problems of metal flow, thermal analysis, distortion and residual stress. Microstructural modelling and prediction of internal damage is either non-existent or still largely at the research stage. A major area for development in industrial modelling is tracking the product state (microstructure or residual stress) through multi-stage processing.

Polymer process modelling has much in common with metals. The use of mould filling software has been routine for many years, while the development of greater microstructural modelling is an area of growing research interest.

As modelling matures in different sectors and the markets grow rapidly, there is a risk that materials process models will be produced with either too little materials expertise, or without adequate validation. The great improvements in user-interfaces also make it easier to generate superficially convincing, but fundamentally flawed, results. Software which is over-sold can lead to rapid disillusionment and set back technology transfer, especially in SMEs.

Independent comparative benchmarking and consultancy in a given sector is therefore essential. It is important for users to understand that no one piece of code can ever solve all problems in a given sector. Standardising code is not desirable, as it is in standardising test methods - the goal should be flexibility, so that individual codes are readily adapted to a wide range of product forms and materials. This requires a major input from software engineering.

Modelling forces plant operators to question their practices and understanding, leading to improved process control and product quality. Modelling of standard tests can initially be as valuable as modelling the process or component in service itself.

Economic considerations are conspicuously lacking in some modelling efforts, but are of paramount importance from the industrial point of view. Many non-modelling functions can be vital in an industrial modelling package: e.g. process-time calculations and cost estimates, and a database of past projects or configurations. Software also offers a means for documenting and interrogating the accumulated empirical know-how of experts.

Modelling has a major role to play in "Design for Manufacture" by bringing processing into design at an appropriate level of complexity. Integration of CAD with relatively simple FE stress analysis and process simulations offers great payoffs in industry. Modelling of component performance will be greatly enhanced in future by coupling CAD and processing simulations to stress analysis. Modelling also plays a role in ensuring materials and processes satisfy the demands of standards and certification procedures.

## Academic modelling

There is potential for greater academic-industrial collaboration on modelling in every industrial sector. Materials modelling with industrial relevance, however long-term, is no less demanding scientifically than purely scientific research modelling. Modelling is often the way in which new scientific challenges are highlighted, and stimulates both theoretical and experimental studies with a more sharply defined focus.

In many academic modelling activities, provision of useful modelling tools for industry is cited as an objective far more frequently than it is in fact achieved in practice. There is little incentive for academics to turn out even demonstrator software, given the nature of the present Research Assessment Exercise. Furthermore, modelling by its very nature is usually a collaborative activity, but the credit and incentives for collaborative research are largely considered to be insufficient.

Universities should not however be spending their time on software packaging. There is perhaps a greater role here for spin-off companies, or intermediate research institutions, which retain close links with the academics, while taking over much of the commercialisation and industrial liaison. There are good European precedents for this approach.

Research models play an important role whether or not the software is commercialised. A balanced view is required, where commercialisation is not deemed to be the only successful outcome of academic modelling research. Some academics express the view that there is now too much pressure to do directly applicable development, rather than research.

Two popular scientific themes in materials modelling are multi-physics modelling and linking length scales. These issues require careful handling, and should not develop into modelling bandwagons. The case for adding greater complexity or making some length-scale connection should be carefully argued, as the "next big challenge" is very dependent on process or material problem.

Atomistic and molecular calculations are making good headway in polymers, following the success of drug simulation for the pharmaceutical industry. Their role in other classes of material and problem is less clear - the best potential appears to be for interfaces and surface behaviour, and for electronic materials. The case is easily over-sold for large-scale metals processing, where in many cases there is little or nothing of industrial use to be gained until meso-macro connections have been made to a much greater level of understanding. Great care is needed in identifying the number of levels of microstructure which play a strong role between atoms and components.

## **Technology transfer**

Most research activity and software development is only accessible to the larger high-technology end of manufacturing industry. To make a significant impact in SMEs, support is needed for: more manpower training, robust well-packaged PC-based software to solve routine first-order problems, more organisations offering advice independently of the software suppliers.

There is a good case for having Centres of Excellence to offer advice and consultancy on modelling, and to act as a channel for technology transfer from universities to industry. Technology transfer, software validation, benchmarking and so on can appear less demanding academically, but nonetheless need enthusiastic academic input. A good compromise is therefore a halfway house, closely linked to a university, in which academics play a part-time role.

Centres should ideally conduct modelling as one of a range of related activities (rather than simply develop or implement software), to maintain a close link with experimental work, and developments in underlying science and research modelling.

There is also great potential for technology transfer in modelling between widely different processes which are not apparently linked in most traditional classification of processes. This arises from the commonality of much of the physical behaviour (e.g. heat transfer, material flow and deformation, microstructure evolution etc.) and software structure (e.g. CAD into FE). Centres currently tend to operate on a sector-by-sector basis, but should be able to exploit these parallels with other processes, crossing traditional boundaries.

A better understanding is needed in both large and small companies of the ways in which the routine use of models can lead to greater efficiency and quality within a manufacturing system.

## **Computational aspects**

Computational power is not an issue except for certain complex 3D processing problems, or the most ambitious research process models embedding multiple levels of physics, or for materials science modelling at the atomistic or molecular scale. The dominant need now is to combine established materials science knowledge with available mechanics and control theory, and thereby target the most productive scientific challenges.

There is a widespread feeling that FE methods are very mature, and that further development would offer little real benefit at present. Problems are limited to niche applications - though there are real needs for codes to be adapted when applied to a class of materials significantly different to those for which the code was initially developed (e.g. mechanics of composites). Some of the national science budget is going on code development which properly belongs to software houses. Much more can be achieved by integrating microstructural modelling with FE.

All thermomechanical materials process modelling encounters problems with interfaces, in particular friction and heat transfer. There is a clear need for a focused research effort on micro-modelling of interfacial conditions, and the coupling of these models to macroscopic FE computations.

Software engineering developments are needed to enable smoother transfer of data from design through to production (CAD - FE mesh - process model - product stress analysis).

### **Data for modelling**

A critical part of any modelling project is establishing from the outset the availability and cost of data, either as input to a model or to validate it and test its sensitivity.

There is a real need for data for processing, but measurement programmes have not always been very successful, or properly validated. While a lot of relevant data will be proprietary and therefore unavailable, there is clearly scope to assemble non-competitive data. Government funded programmes tend to concentrate on techniques for measurement, not assembly of databases. There is a role for trade associations here, or another mechanism is pooling data within a "club" of related industries.

The new DTI programme on measurement of materials parameters for processing (MMP, replacing the former PMP programme) appears now to have taken on board the importance of modelling, including the importance of sensitivity analysis and tuning experimental techniques and precision to the needs of the modeller. Key areas in modelling, such as friction and heat transfer, or the flow behaviour of mushy zones in casting, are well-represented in the new programme.

## **Education and training**

The educational demands on materials-related degree courses in general was highlighted in the Technology Foresight document on Materials. It is important to relate these demands to the view that materials modelling is a key development area. In the UK, almost all modelling groups agree that neither undergraduate nor postgraduate training currently produces enough people able to use and develop modelling tools effectively.

Consideration should be given to developing courses which combine materials science and engineering, numerical methods and software engineering, at undergraduate and postgraduate level. An earlier study concluded that there are several ways of classifying modelling problems in terms of the physics and mathematics of the problem, the type of boundary conditions, and the type of data required. This view of materials process modelling is a useful basis for training process modellers, and could be developed further. Awareness of the industrial and business context of modelling is also an important aspect of process modelling education.

Experienced modellers all say that the principal requirement in a modeller is having the right attitude, i.e. an ability to work in an inter-disciplinary team, an open-minded approach with a gift for lateral thinking, and a clear view that a model is a tool to reach an end rather than an end in itself. This should be reflected in the ways process modelling is taught.

There are many EPSRC initiatives in research training (graduate schools, Teaching Company Schemes, IDGR etc). The role of these schemes could be considered in some depth for materials modelling. Provision of good university education in materials modelling places demands on the expertise of academic staff which cannot currently be met. Consideration also needs to be given to training the teachers of science, engineering and technology to provide sufficient breadth and industrial awareness in university teaching of materials modelling. Post-graduate training and industrial short courses should be co-ordinated at a national level to achieve the breadth required and a balanced view. Centres of excellence could aim to bring together academics from several institutions to deliver this training.

## **Carrying Foresight forward**

Collaboration in materials modelling must be seen at the very least with a European dimension: most UK industry will not hesitate to go to a European university to collaborate if expertise is insufficient in the UK; similarly it is essential for UK universities to be looking to European industry. It has been commented that industrial collaboration in Europe does not gain sufficient recognition in obtaining funding from EPSRC.

It is also important to recognise the level of activity worldwide in materials modelling. An international science-watch aspect is very important in this field - and technology transfer is potentially much more straightforward, as models and data are largely electronic information.

The Foresight recommendation that industry should take the lead in defining research priorities needs some careful consideration in modelling: on the one hand it is apparent that many industries are not sufficiently aware of what modelling can do for their operations (especially in SMEs), so academics have a role to play in promoting modelling in industry; on the other hand, a purely academic lead can mean that pure science or computing is presented as industrially useful, when this is far from the case. As in other areas of research, it is important to support industrially-related modelling research, but also to maintain a solid base of scientific research in materials modelling without undue constraint from industry.

Networking is considered to be important by almost all involved in materials modelling, especially for improving communication between the data gathering, sensor development and modelling communities. The World-Wide Web is not judged by everybody to be a particularly reliable source of data or information, as it is mostly self-publication without screening by referees, but it is increasingly used to assemble software. Consulting the Web is also regarded as time-consuming for little return, but people seem to accept a certain inevitability about making use of it. There is strong support for assembling a directory of information on modelling-related activity in the UK, both on the Web and on a CD for free distribution to a wider industrial audience. The content of the directory must however clearly offer more than the existing general research directories.

It is agreed that there is no real substitute for personal interaction to stimulate collaboration in materials modelling, as in any other field. A popular forum is the one or two-day workshop, covering a well-defined range of modelling activity.

# References

- Ashby M.F. Physical modelling of materials problems. *Materials Science and Technology* 8(2) (1992) 102-111.
- Bailey C., Chow P., Cross M., Fryer Y. and Pericleous K. Multiphysics modelling of the metals casting process. *Proc. Roy. Soc. A* 452, pp.459-486 (1996).
- Bhadeshia H.K.D.H., Mackay D.J.C. and Svensson L.-E. Impact toughness of C-Mn steel arc welds - Bayesian neural network analysis. *Materials Science and Technology* 11(10), pp. 1046-1051 (1995).
- Bratland D., Grong Ø., Shercliff H.R., Myhr O.R. and Tjøtta S. Overview - Modelling of Precipitation in Industrial Processing. *Acta Materialia* 45 (1), p.1-22 (1997)
- Campbell J. and Humphreys C. A framework for the future. *Materials World*, June 1995, p.286-287 (1995).
- Davies C.H.J. Growth of nuclei in a cellular-automata simulation of recrystallisation. *Scripta Materialia* 36(1). pp.35-40. (1997)
- Dreisbach R.L. Working together in the design analysis of transport aircraft structure. *Proceedings of Workshop on "Concurrent Engineering and CALS"*, Royal Aeronautical Society, London, November 1995, pp. 1.1-1.49 (1995)
- Edwards L. and Endean M. (eds.) *Manufacturing with materials*, Materials in Action Series. Butterworth Scientific Ltd, (1990).
- EPSRC (Engineering and Physical Sciences Research Council). The EPSRC Programme 1996-97. April 1996. (1996a)
- EPSRC (Engineering and Physical Sciences Research Council). Response to Foresight. February 1996. (1996b)
- Hollox G.E. The Processing and Engineering Application of Materials. Unpublished report to SERC, provided courtesy of I.Cameron (EPSRC). (1993)
- IBM (International Business Machines Corporation). Technical literature on CATIA Analysis and Simulation Solutions Products. IBM/Dassault Systèmes, Suresnes, France. (1996)
- Ichikawa K., Bhadeshia H.K.D.H. and Mackay D.J.C. Model for solidification cracking in low alloy steel weld metals. *Science and Technology of Welding and Joining*, 1(1), p.43 (1996).
- Institute of Materials. Materials Technology Foresight on Aerospace Structural Materials. Materials Strategy Commission (Institute of Materials), September 1995. (1995)
- Lenau T. and Alting L. Artificial intelligence for process selection. *J. Mechanical Working Technology* 17 (Aug.) (1988) 33-49.

- NPL (National Physical Laboratory). Reliable Data for Process Modelling, NPL leaflet. (1996).
- OST (Office of Science and Technology). Progress through Partnership: Report from the Steering Group of the Technology Foresight Programme. HMSO Publications. (1995a).
- OST (Office of Science and Technology). Progress through Partnership: 10 - Materials. HMSO Publications. (1995b).
- Rappaz M. and Gandin Ch.-A., Probabilistic modelling of the microstructure formation in solidification processes. *Acta metall. mater.* 41(2) (1993) 345-360.
- Rappaz, M., and Kedro M. (eds.). *Proceedings of the General Cost 512 Workshop on Modelling in Materials Science and Processing*, October 1996, Davos, Switzerland (1996).
- Rendigs K.-H., Aluminium Structures Used in Aerospace - Status and Prospects. *Proc. 5th Int. Al Alloy Conf.*, Grenoble, France, July 1996. Vol. 4, p.11 (1996)
- Richmond O., Microstructure-based Modelling of Deformation Processes. *J. Metals.* (1988).
- Richmond O., Materials-based Deformation Process Models. *Proc. Conf. Mathematical Modelling of Metals Processing Operations.* TMS, Palm Springs. (1987).
- Sainfort P., Sigli C., Raynaud G.M. and Gomiero P., Structure and Property Control of Aerospace Alloys. *Proc. 5th Int. Al Alloy Conf.*, Grenoble, France, July 1996. Vol. 4, p.25 (1996)
- Sargent P., Shercliff H.R. and Wood R.L. Modelling Materials Processing, Report for the ACME Directorate of SERC. *Cambridge University Engineering Department Technical Report, CUED/C-MATS/TR206*, October 1993. (1993)
- Wood, R.L. An appraisal of current process modelling technology and a structured view of its potential future progress: part 1 - current technology; part 2 - a structured view. *Processing of Advanced Materials* (1993a).
- Wood, R.L. An inverse thermal field problem based on noisy measurements: comparison of genetic algorithm and sequential function specification method. *Int. J. Computer-Aided Engineering* (1993b).

# APPENDIX

---

## List of people consulted

This is a list of the people who kindly gave their time to answering questions and showing something of their work, either by meeting the author or by correspondence/questionnaire. The views and conclusions represented in this report, however, being distilled from a wide number of opinions, are the responsibility of the author alone.

### Discussions/correspondence

Prof. Mike Ashby	Dept. Engineering, University of Cambridge
Dr. Chris Bailey	Centre for Numerical Modelling and Process Analysis University of Greenwich
Dr. Peter Bate	School of Metallurgy and Materials, University of Birmingham
Dr. David Beveridge	Teesside Laboratories British Steel Technical
Prof. John Beynon	Dept. Mechanical Engineering University of Sheffield
Dr. Steve Brown	Dept. Materials Science, University College of Swansea
Dr. Steve Bull	Dept. of Mechanical, Materials and Manufacturing Engineering University of Newcastle
Mr. Roger Burdett	EPSRC
Prof. Alan Cocks	Dept. Engineering, University of Leicester
Dr. Chris Constantinou	Sowerby Research Centre British Aerospace, Filton

Mr. Adrian Demaid	Faculty of Technology Open University
Dr. Brian Derby	Dept. Science of Materials, University of Oxford
Prof. Russell Evans	Dept. Materials Science, University College of Swansea
Dr. Roman Grzonka	Sowerby Research Centre British Aerospace, Filton
Dr. Richard Hall	School of Manufacturing & Mechanical Engineering, University of Birmingham
Dr. Peter Hartley	School of Manufacturing & Mechanical Engineering, University of Birmingham
Dr. Andrew Howe	Swinden Technology Centre British Steel
Prof. John Humphreys	Manchester Materials Science Centre, University of Manchester & UMIST
Dr. Peter Ingham (and colleagues)	Swinden Technology Centre British Steel
Dr. David Isaacs	Dept. Materials Science, University College of Swansea
Dr. Mark Jolly	Castings Centre, IRC in Materials University of Birmingham
Dr. Dan Kells	Sowerby Research Centre British Aerospace, Filton
Dr. Paul Marshall	Sowerby Research Centre British Aerospace, Filton
Prof. Ron McEwen	Sowerby Research Centre British Aerospace, Filton
Dr. Debravco Nardini	Banbury Laboratory Alcan International
Prof. Trevor Page	Dept. of Mechanical, Materials and Manufacturing Engineering University of Newcastle
Dr. David Petty (and colleagues)	Teesside Laboratories British Steel Technical
Dr. Ian Pillinger	School of Manufacturing & Mechanical Engineering, University of Birmingham
Dr. Ricky Ricks	Banbury Laboratory Alcan International

Dr. Tom Robertson	Teesside Laboratories British Steel Technical
Dr. Jonathan Robinson	Dept. of Materials Science and Metallurgy University of Cambridge
Dr. Steve Rogers	Banbury Laboratory Alcan International
Dr. Philip Sargent	Quillion Systems, Cambridge
Prof. Mike Sellars	Dept. Engineering Materials Sheffield University
Dr. Brian Smith	Teesside Laboratories British Steel Technical
Dr. Julian Spence	Process Modelling Group Rolls Royce
Mr. Paul Spilling	Process Modelling Group Rolls Royce
Dr. Mike Stowell	
Prof. Clive Sturgess	School of Manufacturing & Mechanical Engineering, University of Birmingham
Dr. John Wadsworth	Swinden Technology Centre British Steel
Mr. Peter Warren	Teesside Laboratories British Steel Technical
Dr. Keith Waterson	Banbury Laboratory Alcan International
Dr. Ray Widdowson	Teesside Laboratories British Steel Technical
Dr. Stewart Williams	Sowerby Research Centre British Aerospace, Filton
Mr. Bob Wood	Dept. of Manufacturing Engineering, Loughborough University of Technology
<u>Respondents to questionnaire</u>	
Dr. Chris Bailey	Dept. of Computing and Mathematical Sciences University of Greenwich
Dr. Harry Bhadhesia	Dept. of Materials Science and Metallurgy University of Cambridge
Prof. Alan Bramley	School of Mechanical Engineering University of Bath

Dr. Paul Bristowe	Dept. of Materials Science and Metallurgy University of Cambridge
Dr. Mark Burchell	Dept of Physics University of Kent
Prof. Brian Cantor	Dept. of Materials University of Oxford
Dr. E.A. Colbourn	Oxford Materials Ltd Frodsham
Mr. Phil Costigan	Raychem Swindon
Dr. David Dixon	Sowerby Research Centre British Aerospace, Filton
Dr. Clive Fenn	FlowTech Design Ltd Bolton
Mr. R.A. Ford	IMT Ltd, Bury St Edmunds
Prof. F.P. Glasser	Dept. of Chemistry University of Aberdeen
Dr. Gerhard Goldbeck-Wood	Dept. of Materials Science and Metallurgy University of Cambridge
Dr. Patrick Grant	Dept. of Materials University of Oxford
Dr. Roman Grzonka	Sowerby Research Centre British Aerospace, Filton
Dr. Malcolm Hall	British Polymer Training Association Ltd, Telford
Dr. F. Matthews	Centre for Composite Materials Imperial College, London
Prof. L.N. McCartney	National Physical Laboratory Teddington
Prof. T.C.B. McLeish	IRC in Polymer Science and Technology University of Leeds
Dr. David Porter	Structural Materials Centre DRA Farnborough
Prof. G.D. Price	Dept. of Geological Sciences University College London
Dr. Sally Price	Dept. of Chemistry University College London
Dr. Philippa Reed (and colleagues)	Dept. of Engineering Materials University of Southampton

Dr. Steve Roberts	Dept. of Materials University of Oxford
Mr. Simon Smith	TWI (The Welding Institute) Abington Hall, Cambridge
Prof. Marshall Stoneham	Dept. of Physics University College London
Prof. Ken Thomas	Dept. of Mathematics University of Wales, Aberystwyth
Prof. I.M. Ward	IRC in Polymer Science and Technology University of Leeds
Dr. Eric Wilson	School of Engineering Sheffield Hallam University
Prof. Alan Windle	Dept. of Materials Science and Metallurgy University of Cambridge
Dr. J.R. White	Dept. of Mechanical, Materials and Manufacturing Engineering University of Newcastle
Dr. Yuyuan Zhao	IRC in Materials University of Birmingham