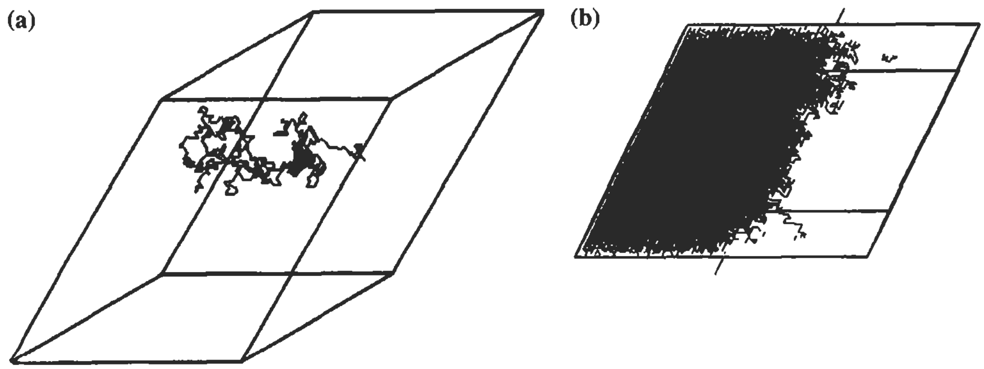

Figure 12.5. (a) Lattice model showing a polymer chain of 200 'beads', originally in a random configuration, after 10,000 Monte Carlo steps. The full model has 90% of lattice sites occupied by chains and 10% vacant. (b) Half of a lattice model containing two similar chain populations placed in contact. The left-hand side population is shown after 50,0000 Monte Carlo steps; the short lines show the location of the original polymer interface (courtesy K. Anderson).

the number of effective 'crossovers' achieved in a given time varies as the square root of the mean molecular weight, and has also allowed strength to be predicted as a function of molecular weight, temperature and time (K. Anderson and A.H. Windle, private communication). The procedure for the MC model involved in this simulation is described by Haire and Windle (2001).

Another family of simulations concerns polymeric fibres, which constitute a major industrial sector. Y. Termonia has spent many years at Du Pont modelling the extrusion and tensile drawing of fibres from liquid solution. A recent publication (Termonia 2000) uses an extreme form of coarse-graining to simulate the process; the model starts with an idealised oblique set of mutually orthogonal straight chains with regular entanglement points. This system is deformed at constant temperature and strain rate, by a succession of minute length increments, moving the top row of entanglement points in the draw direction while leaving the bottom row unmoved. The positions of the remaining entanglement points are then readjusted by an iterative relaxation procedure which minimises the net residual force acting on each site. After each strain increment and complete relaxation, each site is 'visited' by an MC lottery (in the author's words), and four processes are allowed to occur, breakage of interchain bonds, slippage of chains through entanglements, chain breakage and final network relaxation. Then the cycle restarts. All this is done for chains of different lengths, i.e., different molecular weights. The model shows how low molecular weights lead to poor drawability and premature fracture, in accord with experiment. Termonia's extrapolation of this simulation, in the same book, to ultrastrong spider web fibres, where molecular weight *distribution* plays a major part in determining mechanical properties, shows the power of the method.

12.2.3.5 Simulation of plastic deformation. The modelling of plastic deformation in metals presents in stark form the problems of modelling on different length scales. Until recently, dislocations have either been treated as flexible line defects without consideration of their atomic structure, or else the Peierls–Nabarro force tying a dislocation to its lattice has been modelled in terms of a relatively small number of atoms surrounding the core of a dislocation cross-section. There is also a further range of issues which has exercised a distinct subculture of modellers, attempting to predict the behaviour of a polycrystal from an empirical knowledge of the behaviour of single crystals of the same substance. This last is a huge subject (see Section 2.1.6), and I can do no more here than to cite a concise coverage of the issues in Chapter 17 of Raabe's (1998) book and also to refer to *the* definitive treatment in detail, representing many years of work (Kocks *et al.* 1998).

Very recently, the modelling of plastic deformation in terms of the motion, interaction and mutual blocking of dislocations moving under applied stress has entered the mesoscale. Two papers have applied MD methods to this task; instead of treating dislocations as semi-macroscopic objects, the motion of up to 100 million individual atoms around the interacting dislocation lines has been modelled; this is feasible since the timescale for such a simulation can be quite brief. One paper is by Bulatov *et al.* (1998), the other by Zhou *et al.* (1998); each has received an illuminating discussion in the same issues of their respective journals. These two studies follow a first attempt by L.P. Kubin and others in 1992. As P. Gumbsch points out in his discussion of the Zhou paper, these atomistic computations generate such a huge amount of information (some 10^4 configurations of 10^6 atoms each) that "one of the most important steps is to discard most of it, namely, all the atomistic information not directly connected to the *cores* of the dislocations. What is left is a physical picture of the atomic configurations in such a dislocation intersection and even some quantitative information about the stresses required to break the junction". This kind of information overload is a growing problem in modern super simulation, and knowing what to discard, as well as turning pages of numbers into readily assimilable visual displays, are central parts of the simulator's skill.

Baskes (1999) has discussed the "status role" of this kind of modelling and simulation, citing many very recent studies. He concludes that "modelling and simulation of materials at the atomistic, microstructural and continuum levels continue to show progress, but prediction of mechanical properties of engineering materials is still a vision of the future". Simulation cannot (yet) do everything, in spite of the optimistic claims of some of its proponents.

This kind of simulation requires massive computer power, and much of it is done on so-called 'supercomputers'. This is a reason why much recent research of this kind has been done at Los Alamos. In a survey of research in the American national laboratories, the then director of the Los Alamos laboratory, Siegfried Hecker (1990) explains that the laboratory "has worked closely with all supercomputer vendors over the years, typically receiving the serial No. 1 machine for each successive model". He goes on to exemplify the kinds of problems in materials science that these extremely powerful machines can handle.

12.3. SIMULATIONS BASED ON CHEMICAL THERMODYNAMICS

As we have repeatedly seen in this chapter, proponents of computer simulation in materials science had a good deal of scepticism to overcome, from physicists in particular, in the early days. A striking example of sustained scepticism overcome, at length, by a resolute champion is to be found in the history of CALPHAD, an acronym denoting CALculation of PHAse Diagrams. The decisive champion was an American metallurgist, Larry Kaufman.

The early story of experimentally determined phase diagrams and of their understanding in terms of Gibbs free energies and of the Phase Rule was set out in Chapter 3, Section 3.1.2. In that same chapter, Hume-Rothery's rationalisation of certain features of phase diagrams in terms of atomic size ratios and electron/atom ratios was outlined (Section 3.3.1.1). Hume-Rothery did use his theories to predict limited features of phase diagrams, solubility limits in particular, but it was a long time before experimentally derived values of free energies of phases began to be used for the prediction of phase diagrams. Some tentative early efforts in that direction were published by a Dutchman, van Laar (1908), but thereafter there was a void for half a century. The challenge was taken up by another Dutchman, Meijering (1957) who seems to have been the first to attempt the calculation of a complete ternary phase diagram (Ni–Cr–Cu) from measured thermochemical quantities from which, in turn, free energies could be estimated. Meijering's work was particularly important in that he recognised that for his calculation to have any claims to accuracy he needed to estimate a value for the free energy (as a function of temperature) of face-centred cubic chromium, a notional crystal structure which was not directly accessible to experiment. This was probably the first calculation of the lattice stability of a potential (as distinct from an actual) phase.

At the time Meijering published his research, Larry Kaufman was working for his doctorate at MIT with a charismatic steel metallurgist, Professor Morris Cohen, and they undertook some simple equilibrium calculations directed at practical problems of the steel industry. From the end of the 1950s, Kaufman directed his efforts at developing these methods, sustained by two other groups, one in Stockholm, Sweden, run from 1961 by Mats Hillert and another in Sendai, Japan, led by T. Nishizawa. Hillert and Kaufman had studied together at MIT and their interaction over the years was to be crucial to the development of CALPHAD.

At a meeting at Battelle Memorial Institute in Ohio in 1967, Kaufman demonstrated some approximate calculations of binary phase diagrams using an ideal solution model, but met opposition particularly from solid-state physicists who preferred to use first-principles calculations of electronic band structures instead of thermodynamic inputs. For some years, this became the key battle between competing approaches. At about this time, Kaufman began exchanging letters with William Hume-Rothery concerning the best way to represent thermodynamic equilibria. Thereupon, Hume-Rothery, in his capacity as editor of *Progress in Materials Science*, invited Kaufman to write a review about lattice stabilities of phases, which appeared (Kaufman 1969) shortly after Hume-Rothery's death in 1968. Shortly before his death, Hume-Rothery had written to Kaufman to say that he was "not unsympathetic to any theory which promises reasonably accurate calculations of phase boundaries, and saves the immense amount of work which their experimental determination involves", but that he was still sceptical about Kaufman's approach. This extract comes from a full account of the history of CALPHAD in Chapter 2 of a recent book (Saunders and Miodownik 1998). In his short overview, Kaufman took great trouble to counter Hume-Rothery's reservations, and he also gave a fair account of the competing band-theoretical approaches. The imperative need to account for the competition in stability between alternative phases, actual and potential, was central to Kaufman's case.

For the many ensuing stages in CALPHAD's history, including the incorporation of CALPHAD Inc. in 1973, and the practice of organising meetings at which different approaches to formulating Gibbs energies could be reconciled, Saunders and Miodownik's history chapter must be consulted. Effective international cooperation got under way in 1973, with involvement of a number of national laboratories, and numerous published computer codes from around the world such as Thermocalc and Chemsage are now in regular use. From 1976 on, physicists were encouraged to attend CALPHAD meetings in order to assess the feasibility of merging data obtained by thermochemistry with those calculated by first-principles electron-theory methods (Pettifor 1977). CALPHAD's own journal began publication in 1977. Kaufman is still, today, a key participant at the regular CALPHAD meetings.

Kaufman and Bernstein (1970) brought out the first book on phase diagram calculations; there was not another comprehensive treatment till Saunders and Miodownik's book came out in 1998. This last covers the ways of obtaining the thermodynamic input data, ways of dealing with complications such as atomic

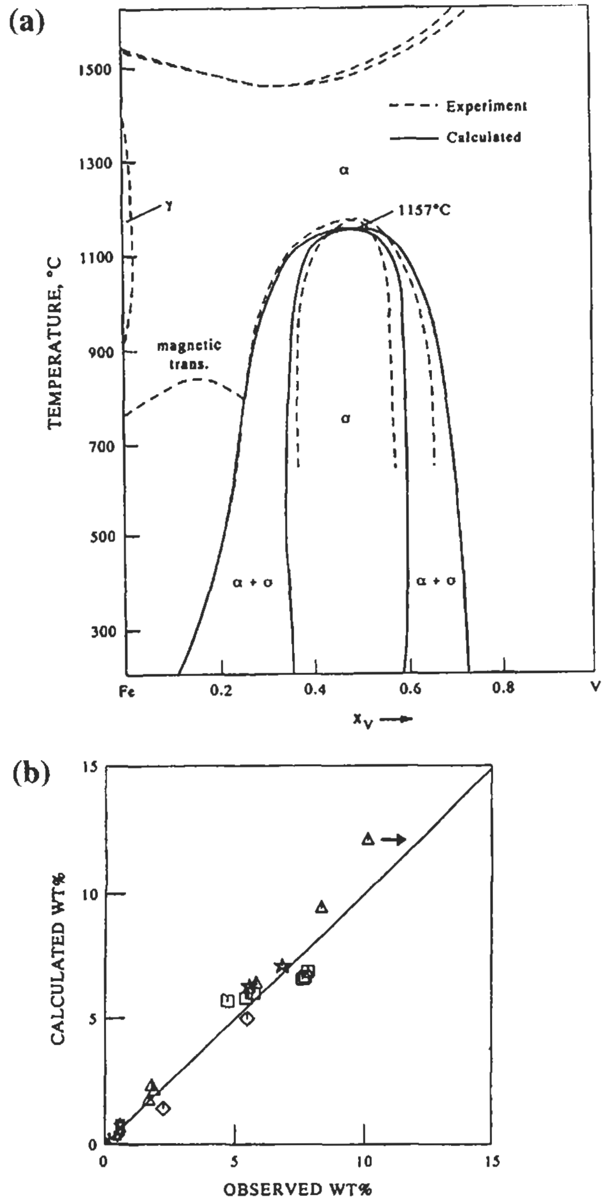

Figure 12.6. (a) Calculated (α + σ) phase boundary for Fe–V together with experimental boundaries (After Spencer and Putland 1973). (b) Comparison between calculated and experimental values of the concentration of Al, V and Fe in the two phases in Ti–6Al–4V alloy (after Saunders and Miodownik 1998).

ordering and ferromagnetism, and (in particular) many forms of application of CALPHAD. It also describes the crucial methods of critically *optimising* thermodynamic data for incorporation in internationally agreed databases. Figure 12.6(a) shows an early example of a simple binary phase diagram obtained by experiment together with calculated phase boundaries. Figure 12.6(b) shows a plot of observed versus calculated solute concentrations in a standard titanium alloy. It has been an essential part of the gradual acceptance of CALPHAD methods that theory and experiment have been shown to agree well, and progressively better so as methods improved. Indeed, *in all computer modelling and simulation, confidence can only come gradually from a steady series of such comparisons between simulation and experiment.*

Even when the CALPHAD approach had been widely accepted as valid, there was still the problem of the reluctance of newcomers to start using it. Hillert (1980) proposed looking at thermodynamics as a game and to consider how one can learn to play that game well. He went on: "For inspiration, one may first look at another game, the game of chess. The rules are very simple to learn, but it was always very difficult to become a good player. The situation has now changed due to the application of computers. Today there are programmes for playing chess which can beat almost any expert. It seems reasonable to expect that it should also be possible to write programmes for 'playing thermodynamics', programmes which should be almost as good as the very best thermodynamic expert." In other words... for novices, tried and tested commercial software, whether for thermodynamics or for MC or MD, should take the sting out of taking the plunge into computer simulation, and perhaps in the fullness of time such simulations will move out of specialised journals and coteries of specialists and find their way increasingly into mainline journals, and students with first degrees in materials science will be entirely at ease with this kind of activity. Perhaps we are already there.

Today, thermodynamic simulation has broadened out far beyond the calculation of binary and ternary (and even quaternary) phase diagrams. For instance, as explained in the last chapter of Saunders and Miodownik's book, methods have recently been developed to combine diffusional simulations with phase stability simulations in order to obtain estimates of the kinetics of phase transformation. A recent text issued by SGTE, the Scientific Group Thermodata Europe (Hack 1996) includes 24 short chapters instancing applications, in particular, to processing issues. Two examples from Sweden, relating to solidification, include the calculation of solidification paths for a multicomponent system and (severely practical) calculations directed towards the prevention of clogging by premature freezing in a continuous casting process. Another chapter discusses the formulation of a Co–Fe–Ni binder phase for use with a dispersion of tungsten carbide 'hard metal'. A chapter by Per Gustafson in Sweden hinges on computer development of a high-speed (cutting) steel. This last application is reminiscent of a protracted programme of research at Northwestern University (where materials science started in 1958) by Gregory Olson (e.g. Kuehmann and Olson 1998) to design steels for specially demanding purposes by a sophisticated computer-optimisation program, including extensive use of CALPHAD; some further remarks about this program can be found in Section 4.3.

Very recently, a very detailed report from two groups attending a 1997 meeting on 'Applications of Computational Thermodynamics' has been published (Kattner and Spencer 2000) with presentations of many applications to practical problems, with emphasis on processing methods, including processing of semiconductors and microcircuits. One process modelled here is the deposition of a compound semiconductor from an organometallic precursor, a 'soft chemistry' approach discussed in the preceding chapter.

The CALPHAD approach has been treated here at some length because its history illustrates the strengths and limitations of computer modelling and simulation. The strengths clearly outweigh the limitations, and this is becoming increasingly true throughout the broad spectrum of applications of computers in materials science and engineering.

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Chapter 13

The Management of Data

Chapter 13

The Management of Data

13.1. THE NATURE OF THE PROBLEM

As I write this, one of my grandchildren has just asked me which is the 'heaviest' metal. I did not have any listing available at home, and I guessed uranium or tungsten. My grandson Daniel preferred to believe that gold was the heaviest, i.e., densest. Now, sitting in my office, I cast about for a convenient listing of densities, and chose the *Metals Reference Book*, fourth edition, 1967, volume 3. It turns out that neither my grandson nor I were quite right: gold and tungsten have virtually the same density, uranium is marginally less dense, but several noble metals (platinum, osmium, and others) are even denser. Of course, I had to skim the whole column listing densities of pure metals and look for the highest value; with a suitable computerised listing, I could have asked the computer "Which of these elements is densest?" – if a computerised way of putting such a question is available – and (perhaps) got an answer in the blink of an eye. All this is a very minor example of the problems of data retrieval.

Of course, densities of pure metals do not change over time, though the available precision may improve a little over the decades. However, many more complex data do change significantly as new experiments are done, and new materials or material systems come along constantly and so entirely new data flood the literature. Materials scientists, like chemists, physicists and engineers, need means of finding these. Those means are called *databases*. This brief chapter surveys how databases are assembled and used, with special attention to materials.

13.2. CATEGORIES OF DATABASE

13.2.1 Landolt–Börnstein, the **International Critical Tables** *and their successors*

Initially, natural philosophers communicated by letter, and in this way measurements of physical and chemical quantities were slowly spread. Then scientific journals began to develop, slowly at first; 200 years ago, there were some 50 of these in the world; data were then spread through journals, for instance, the *Philosophical Transactions of the Royal Society of London*. Attempts to gather scattered data in lists began in earnest in 1883, when Hans Heinrich Landolt and Richard Börnstein in Germany published the first volume of their *Physikalische-Chemische Tabellen*, running to 261 pages. This was well received, and up to 1950, 25 further volumes appeared with broad titles such as *Crystals*, *Fusion Equilibria and Interfacial Phenomena*, *Optical Constants*. The 26 volumes came out in six successive editions until 1969, whereupon the publisher, Springer, decided to change to a more flexible form and started the *New Series*, devoted to a great variety of specialised themes. 129 volumes and subvolumes are listed in the comprehensive 1996 catalogue, with several more planned, and in 2000 all of these were available on the internet, and access was offered free of charge until the entire *New Series*, some 140,000 pages, is on line. Many of the 129 volumes were a long way from relevance to materials – for instance, some are devoted to astronomy – but quite a number are directly related to MSE. This series is unique in its longevity and consistency.

By way of example, Volume 26 in Group III (Crystal and Solid State Physics) is devoted to *Diffusion in Solid Metals and Alloys*; this volume has an editor and 14 contributors. Their task was not only to gather numerical data on such matters as self- and chemical diffusivities, pressure dependence of diffusivities, diffusion along dislocations, surface diffusion, but also to exercise their professional judgment as to the reliability of the various numerical values available. The whole volume of about 750 pages is introduced by a chapter describing diffusion mechanisms and methods of measuring diffusivities; this kind of introduction is a special feature of "Landolt–Börnstein". Subsequent developments in diffusion data can then be found in a specialised journal, *Defect and Diffusion Forum*, which is not connected with Landolt–Börnstein.

Other early tabulations of numerical data were the French *Tables Annuelles de Constantes et Données Numériques* which appeared for some decades after 1920, and the British *Tables of Physical and Chemical Constants*, masterminded by the National Physical Laboratory and known affectionately as "Kaye and Laby" after the editors, which appeared annually in single volume form from 1911 to 1966. These last two, like Landolt–Börnstein, appeared regularly, in successive editions.

Something rather different was the set of 7 volumes of the *International Critical Tables* masterminded by the International Union of Pure and Applied Physics, edited by Edward Washburn, and given the blessing of the International Research Council (the predecessor of the International Council of Scientific Unions, ICSU). This appeared in stages, 1926–1933, once only; when Washburn died in 1934, "the work died with him". This last quotation comes from a lively survey of the history of ICSU (Greenaway 1996); this book has an entire chapter devoted to "Data, and Scientific Information".

It was not until the mid-1960s that Harrison Brown (later ICSU President) called attention to the absence of any successor to the *International Critical Tables*, and was asked by ICSU to make recommendations. This led to ICSU's creation of *CODATA*, following on from ICSU's earlier World Data Centers, devoted to specific sciences such as metereology. This body is more of a gadfly and organiser than publisher of databases, and for example by 1969 it had published an "International Compendium of Numerical Data Projects", and set up a task group on computer usage. *CODATA* became closely involved with the National Academy of Sciences in Washington, DC. In 1984, ICSU created another body, the International Council for Scientific and Technical Information, ICSTI, to be devoted to getting databases to the right user. This is, and has long been, a central problem, because there are now so many databases scattered around the world and most materials scientists know only a very few of them.

The *Metals Reference Book*, mentioned at the beginning of this chapter, published in Britain in successive editions from 1949, and edited by a metallurgist, C.J. Smithells, is a good example of a specialised database kept up to date by periodic new editions. It eventually extended to well over 1000 pages. A somewhat similar compilation focused on polymers is D.W. van Krevelen's book, *Properties of Polymers*, already mentioned in Chapter 8. This more discursive book is now in its third edition, 1990. An example of an even more specialised database is a book by R. Hultgren and 4 others, *Selected Values of the Thermodynamic Properties of the Elements* (American Society for Metals, 1973), which was of great importance, inter alia, for the early efforts in calculation of phase diagrams (see Section 12.3). A more recent compilation of measurements of high-temperature thermodynamic quantities for alloys, measured by high-temperature calorimetry and also valuable for the calculation of phase diagrams, is by Kleppa (1994).

For many materials scientists *the* database for which they automatically reach when a problem arises like the one with which I opened this chapter is the *Handbook of Chemistry and Physics*, now in its 81st edition, with over 2500 pages of densely packed information. This Handbook was first published in 1914 (a few years were missed because of wars), at the instigation of Arthur Friedman, a mechanical engineer and entrepreneur; one of his companies was the Chemical Rubber Company, CRC, in Cleveland, Ohio, which supplied laboratory items in rubber. The CRC published the Handbook from the start, and still does... hence the Handbook's nickname, *The Rubber Bible*. In the early years, Friedman used the *Handbook* as a promotional device for the sale of such items as rubber stoppers.

Information about this splendid compilation came to me from a chemist, Robert Weast (1985), who was editor from 1952 until 1988... 37 years! He also informed me that the creation (jointly by the American Chemical Society and the American Institute of Physics) of the *Journal of Physical and Chemical Reference Data*, which began publication in 1972, was encouraged by the results of a survey which indicated how widely the 'Rubber Bible' was used. Weast describes this journal as "a truly outstanding source of critically evaluated data". In saying this, he underlined the crucial role of editors' and contributors' critical judgment in selecting data for such compilations. David Lide, the editor of the journal, in 1989 succeeded Robert

Weast as editor of the *Rubber Bible*. Although the *Rubber Bible* is not primarily addressed to materials scientists, yet it has proved of great utility for them.

Database construction has now become sufficiently widespread that the ASTM (the American Society for Testing and Materials... a standards organisation) has issued a manual on the building of databases (ASTM 1993); it incorporates advice on computer practice.

An interesting question is what motivates researchers to choose a particular substance for precise measurement of some physical, chemical or mechanical characteristic. I consulted a well-known physicist, Guy White, who works for the Division of Applied Physics of CSIRO in Australia (White 1991). He is concerned with thermophysical measurements, thermal conductivity and thermal expansion in particular. He told me that his choice of materials for thermophysical measurements "were probably dictated by a combination of curiosity, availability and 'simplicity' plus, when opportunity offered, the benefit of a chat with an interested theorist". For instance, the availability of large crystals of certain substances from a British firm prompted their use for thermal expansion measurements. It went further than that, indeed. As White pointed out, "many dilatometers in common use have significant systematic errors in determining linear thermal expansion as evidenced by round-robin measurements on reproducible materials". So high-quality reference materials are needed to check and calibrate precision dilatometers; substances like oxygen-free copper and semiconductor-grade silicon were used for that purpose. Similar round-robin measurements of the lattice parameter of semiconductor-grade silicon powder were used many years ago to test the reliability of different X-ray diffraction instruments and to compare the accuracy of photographic and direct measurement methods. This kind of procedure also picks out the most conscientious operators.

13.2.2 Crystal structures

Crystal structure determination began, as we saw in Chapter 3, in 1912, and was initially rather slow to get under way. By 1929, however, enough crystal structures had been determined to stimulate the creation of a specialist journal, *Strukturbericht*, which continued after the War and until the mid-1980s as *Structure Reports*, published by the International Union of Crystallography. There were also compendia of crystal structures in book form, the best known being a series of books by R. Wyckoff, *The Structure of Crystals*, which began to appear in 1931. Many metallic crystal structures were included in the *Metals Reference Book*. Other specialised books appeared, for instance *Crystal Data*, intended primarily for mineralogists, and the *Powder Diffraction File* in its many successive formats, which listed the lattice spacings and intensities of the lines in powder diffraction patterns from many different substances.

Structure Reports were eventually replaced by structural databases "as curators of the world's primary crystal structure data". This description comes from a splendid overview of "The Development, Status and Scientific Impact of Crystallographic Databases" by Allen (1998). According to Allen, in 1998 the five principal crystallographic databases included about 288,000 entries. Of these, more than two thirds were organic crystal structures, proteins and nucleic acids, some exceedingly complex, the majority included in the Cambridge Crystallographic Database (which got under way in the late 1960s). Two other databases (Inorganic Crystal Structure Database, and CRYSTMET) deal with inorganic and specifically metallic crystal structures (including intermetallic compounds). Allen discusses in some detail the difficult but indispensable task of "validating" crystal structures and bond lengths; inter alia, this involves seeking out simple typesetting errors in the accounts of primary data. The Cambridge database is used extensively by biochemists and, particularly, pharmaceutical firms engaged in drug development: secondary data on bond lengths and interbond angles can prove very useful. These "research applications" are discussed in detail by Allen.

Another recent database, still in evolution, is the Linus Pauling File (covering both metals and other inorganics) and, like the Cambridge Crystallographic Database, it has a "smart software part" which allows derivative information, such as the statistical distribution of structures between symmetry types, to be obtained. Such uses are described in an article about the file (Villars *et al.* 1998). The Linus Pauling File incorporates other data besides crystal structures, such as melting temperature, and this feature allows numerous correlations to be displayed.

13.2.3 Max Hansen and his successors: phase diagram databases

In 1936, Springer in Berlin published a book by a German metallurgist, Max Hansen, which was devoted to a critical assembly of known binary metallic phase diagrams (Hansen 1936). We saw in Chapter 3 that the accurate determination of phase diagrams, such as Fe–C and Cu–Sn, began at the end of the 19th century and so Hansen's pathbreaking book brought together some 40 years' research. The book covered 828 systems and contained 456 phase diagrams, with about 5500 references to the literature. This at once shows that there were several references for each system about which enough was known to publish a diagram. It was Hansen's innovation to exercise his critical faculty on the many instances where different investigators differed as to a liquidus, solidus, eutectic, peritectic, eutectoid or peritectoid temperature, or compositions of solid solutions or eutectic mixtures. His diagrams were 'optimised' diagrams. After the War, Hansen's book was revised (with the help of a coauthor, K. Anderko), translated into English and published in America (Hansen and Anderko 1958). Now there were 1382 systems and 750 diagrams. Some diagrams were buttressed by more than 100 references, with many explicit critical judgments as to the most reliable values of disputed quantities. My personal copy of this book, which I was given as a gift in 1958, has almost fallen apart from frequent use. Subsequently, there were two addendum volumes, in 1965 and 1969, including many revised and improved diagrams.

The crucial role that phase diagrams play in materials science, and the consequential need for compilations like Hansen's, has been memorably portrayed in a lecture by Massalski (1989).

From 1977, the GE Corporate Research Center in New York State began its own private collection of binary metallic phase diagrams, and from 1990 Massalski in Pittsburgh began editing a series of such assessments for the American Society of Metals (now ASM International). Later, he extended his remit to ternary systems. Earlier, in England, Hume-Rothery and his pupil Raynor had brought out, through the Institute of Metals, a number of individual critically assessed phase diagrams for the most important binary systems. There has also been a variety of Russian compilations.

From 1988, Effenberg in Stuttgart, Germany, began the enormous task of masterminding the publication of optimised *ternary* metallic phase diagrams. At the time of writing, some 3500 systems have been scrupulously covered in 18 volumes, and there is still far to go. In 1995, Villars and colleagues brought out a rival ternary compilation which included even more systems.

Further, since 1993, Effenberg has edited the "Red Book", annual summaries of developments in the world literature of phase diagrams.

In 1986, APDIC, the Alloy Phase Diagram International Commission, with the participation of 18 national bodies, was set up "to safeguard the quality of phase diagram evaluations and to provide globally the best possible coordination of the major phase diagram projects". This phrasing is taken from a short article by Effenberg (2001) which provides a complete listing, with bibliographic details, of all the various compilations, and also goes out of its way to emphasise how small a proportion of all possible ternary systems (not to mention quaternaries) have been determined (even partially).

This 66-year programme, to date, of phase diagram evaluation and publication is probably the most judgment-intensive operation ever undertaken in the history of materials science. Reliability, reproducibility and accuracy must all be assessed, and moreover some detailed features of phase diagrams as published are often inconsistent with elementary thermodynamic principles: Okamoto and Massalski (1993) have provided guidelines for avoiding this kind of error. Usually, the many stages of optimising a phase diagram and resolving disparities between different experimenters are passed over in silence. To get an idea of the complexity of the process, a paper by Murray (1985) about the steps in the optimisation of the Cu–Ti phase diagram can be recommended; here, both direct experiment and the result of CALPHAD theory are brought together and assessed.

In addition to all the metallic phase diagrams, a series of volumes devoted to ceramic systems have been published since 1964 by the American Ceramic Society and is still continuing. The original title was *Phase Diagrams for Ceramists*; now it is named *Phase Equilibria Diagrams*. Some 25,000 diagrams, binary and ternary mostly, have been published to date. There is no compilation for polymeric systems, since little attention has been devoted to phase diagrams in this field up to now.

In addition to printed compilations, more and more of the information is available on CD-ROM and latterly also on-line on the internet. This last is a feature of the service provided by MSI, Materials Science International Services in Stuttgart. This organisation, under the working name of MSIT® Workplace (http://www.msiwp.com), provides information on the entire corpus of phase diagram compilations.

It is a reflection on present-day priorities in industry that the research laboratory of a great company, Metallgesellschaft in Frankfurt-am-Main, Germany, where Hansen began work on his epoch-making book, was closed down a few years ago to save money. This laboratory was initially directed, from 1918 onwards, by Jan Czochralski, the Pole whom we met in Section 4.2.1 and who gave his name to the present-day process for growing silicon crystals, and subsequently by Georg Sachs and, after he had been driven from Germany by the Nazis in 1935, by Erich Schmid, all highly distinguished figures. The manifold achievements of the laboratory are described in a book issued on the occasion of the company's centenary, when the laboratory was still going strong (Wassermann and Wincierz 1981).

A long history of distinguished contributions does not suffice, nowadays, to save a research institution from casual destruction.

13.2.4 Other specialised databases and the use of computers

This chapter has only scratched the surface of the multitude of databases and data reviews that are now available. For instance, more than 100 materials databases of many kinds are listed by Wawrousek *et al.* (1989), in an article published by one of the major repositories of such databases. More and more of them are accessible via the internet. The most comprehensive recent overview of "Electronic access to factual materials information: the state of the art" is by Westbrook *et al.* (1995). This highly informative essay includes a 'taxonomy of materials information', focusing on the many different property considerations and property types which an investigator can be concerned with. Special attention is paid to mechanical properties. The authors focus also on the *quality and reliability of data*: quality of source, reproducibility, evaluation status, etc., all come into this, and alarmingly, they conclude that numerous databases on offer today "consist wholly or in part of data that would not even meet the criteria for 'limited use'." They home in on the many on-line databases accessible through STN International, a scientific and technical information network. In fact, there are a number of organisations worldwide, most connected to the internet, which merge a number of independent databases; the Förderverein Werkstoffdokumentation in Germany is another such. ASM International has recently issued a Directory of Materials Property databases (ASM 2000).

One feature discussed by Westbrook *et al.* is the nature of the enquiries that a database can handle... i.e., the quality of its associated software. One example is 'range searching', finding all materials that have values of a particular property in a specified numerical range. This aspect of using databases has recently been examined critically, in two linked papers, by Ashby (1998) and by Bassett *et al.* (1998). For instance, different *categories* of materials have different ranges of value of the thermal expansion coefficient (p. 202). The ranges for ceramics and glasses (small values) do not overlap with the range for polymers (large values). Ashby's comment on this is: "Correlations exist between the values of mechanical, thermal, electrical and other properties which derive from the underlying physics of bonding and packing of atoms. Some of these correlations have a simple theoretical basis and can be expressed as dimensionless groups with much narrower value ranges; they allow a physically based check on property values and *allow some properties to be estimated when values for others are known*" (my italics). The second paper shows how missing data can be estimated by using these principles.

Ashby, some years ago, produced a computerised database called the *Materials Selector* (CMS 1995) which allows the best material to be selected for a particular application with combined criteria (as it might be, least weight and stiffness in a certain range). The ideas which led to this were presented in a book (Ashby 1992). John Rodgers, who operates the CRYSTMET crystallographic database for metals, is now planning to create a database for unfamiliar materials, using the CMS environment and information in CRYSTMET, incorporating a range of calculated or estimated physical property values. It begins to look as though data estimation using information in databases may become a new, distinct activity within materials science and engineering. In fact, the process already has a name – *datamining*. According to John Rodgers, this means "the extraction of implicit, previously unknown and potentially useful information from data" (Rodgers 1999).

Materials selection is as much an art as a rigorous science, and another computational approach to it, based on ideas of artificial intelligence, has been proposed by Arunachalam and Bhaskar (1999). They call their approach "bounded rationality" and exploit it to analyse the background to some notorious disasters based on material failure. We can always learn from failure as well as from success.

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Chapter 14

The Institutions and Literature of Materials Science

Chapter 14

The Institutions and Literature of Materials Science

14.1. TEACHING OF MATERIALS SCIENCE AND ENGINEERING

The emergence of university courses in materials science and engineering, starting in America in the late 1950s, is mapped in Section 1.1.1. The number and diversity of courses, and academic departments that host them, have evolved. An early snapshot of the way the then still novel concept of MSE was perceived by educators, research directors and providers of research funds can be found in an interesting book (Roy 1970) in which, for example, a panel reported that a representative of the GE Company "stressed that his company regards the university as a provider of people and not as an institution which supplies all of the solutions to industry's materials problems. The university should train both materials scientists and engineers, should clearly recognise the difference between these two groups, and should provide the basis for interdisciplinary cooperation." Rustum Roy, the editor of that volume, repeatedly called for just such interdisciplinary cooperation on campus; the high point of his campaign was a paper published in 1977 (Roy 1977). He has done much to bring about just such interdisciplinarity at his own university, Pennsylvania State University, which for many years has hosted an interdisciplinary Materials Research Laboratory of the kind whose history is outlined in Section 1.1.3. His role in creating the Materials Research Society was similarly motivated.

The present situation, both in the US and elsewhere, is examined in a recent survey article (Flemings and Cahn 2000). In the United States, the number of core MSE departments (i.e., independent university departments granting bachelor through doctorate degrees) in 1999 was 41. On top of that, 14 departments are still specific to particular categories of materials, and another 41 are either joint with other disciplines that are peripheral to MSE, or are wholly embedded in departments of other disciplines, such as mechanical or chemical engineering. So, merged or embedded departments are as numerous as independent departments. After a sharp peak in 1982, the number of students granted bachelor's degrees in the US specifically in materials or metallurgy declined somewhat, stabilising at $\approx$1200 per annum in the 1990s. The number of faculty members in MSE departments in 1997 was estimated at 625 (Flemings 1999).

In England (excluding Scotland, Wales and Northern Ireland), there were 21 mainline MSE departments in 1998; Fig. 9.4 (Chapter 9) shows plots of student numbers in the US. On the continent of Europe, where institutes and not full departments are the organisational rule, it is much more difficult to pick out those institutes which are properly described as being in the MSE mainline; an attempt by a range of national societies to list appropriate university institutes has led to numbers ranging from 79 in Germany, via 48 in France to only 4 in Sweden... but many of the institutes listed are in fields which are peripheral to, or barely connected with, MSE. In some universities on the continent, a number of institutes are combined into a materials department. To pick just one example, at the eminent Eidgenössische Technische Hochschule in Zürich, Switzerland, the following institutes (or groups) are currently combined: biomechanics; biomedical engineering; metals and metallurgy; metallic high-performance materials (the distinction between these last two is typical of continental modes of organisation); nonmetallic inorganic materials; polymer chemistry; polymer physics; polymer technology; supramolecular chemistry; surface science and technology. Thus, here semiconductors have been hived off to another department.

Fig. 14.1 shows an impressionistic 'ternary diagram' showing the emphasis on three broad fields relevant to MSE at a range of German universities that prepare students in the study of materials. If one thing is crystal clear, it is that there is no one ideal way of teaching MSE laid up in heaven, and the example of the Swiss department indicates that there is much scope for variety.

In spite of statistical problems, two things are clear from a close examination of student numbers in various countries and institutions: MSE courses are burgeoning, and the best mainline departments are going from strength to strength. However, some of the weaker departments/institutes (those with relatively few students) are being forced by resolute academic deans into marriages with quite distinct disciplines – which (experience suggests) can be a precursor of brain death – or being closed down altogether.

Flemings (1999) reflected under the title "What next for departments of materials science and engineering?" A particularly interesting feature of his paper is a comparison of the characteristics and activities of a class of students who graduated with metallurgy degrees from M.I.T. (Flemings's university) in 1951, with those of another class who graduated in MSE in 1991. In each case, statistics were collected 7 years after graduation; not all students responded (See Table 14.1).

The most striking features, apart from the sharp drop in fecundity, are the large numbers of graduates who went on to obtain business qualifications (Masters of Business Administration, MBAs); the fact that in 1958, working in metallurgy and in engineering seems to have been synonymous in the eyes of respondents, but not so in 1998; the drastic fall in the numbers who gave research and development as their current métier, in spite of a sharp rise in those taking advanced degrees; and the fact that, around the age 30, *none* of the 1998 respondents had become university faculty.

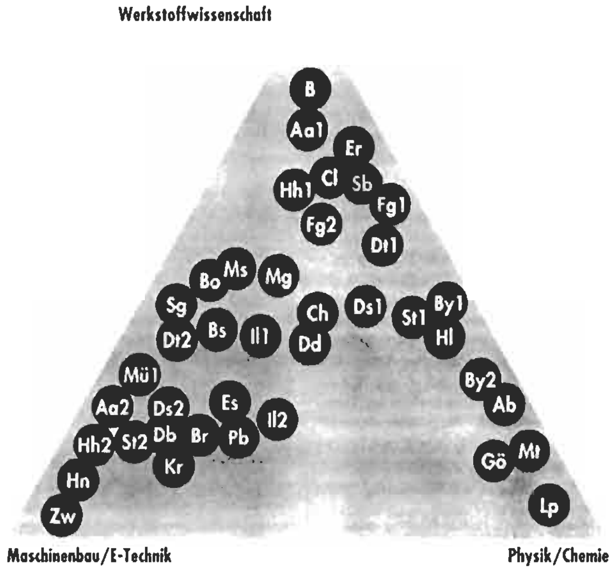

Figure 14.1. Estimated emphasis on three broad fields – Werkstoffwissenschaft = materials science; Maschinenbau/E-technik = mechanical and electrical engineering; Physik-Chemie = physics and chemistry – in MSE education at various German universities from (DGM 1994).

Table 14.1. Particulars of two graduating M.I.T. classes, 7 years after graduation.

	Class of 1951 (%)	Class of 1991 (%)
With advanced degrees	37	64
With MBAs	0	43
Working in metallurgy	89	14
Working in engineering	89	43
University faculty	19	0
In R&D, including faculty	48	14
Married	96	62
Mean number of children per graduate	1.8	0.1

As Flemings points out, compared with the middle of the twentieth century, MSE departments now have to prepare their students for quite different professional lives. The key question that seems to arise from these figures is: Do university departments put too much emphasis on research? And yet, before we conclude that they do, we must remember that it is widely agreed that research is what keeps university faculty alert and able to teach in an up-to-date way. It may well be that what students currently want, and what the health and progress of MSE demands, are two distinct things.

A danger in the increasing mergers of MSE departments with departments of mechanical engineering and chemical engineering in particular is that engineers are in general wedded to a continuum approach to matter while MSE people are concerned with atomic, crystallographic and micro-*structures*... the last of these particularly. If that aspect of materials science is sidelined or abolished, then its practitioners lose their souls.

The key justification of the whole concept of MSE, from the beginning, has been the mutual illumination resulting from research on different categories of materials. The way I worded this recognition in my editorial capacity, writing the Series Preface for the 25 volumes of *Materials Science and Technology*, published between 1991 and 2000, was: "Materials are highly diverse, yet many concepts, phenomena and transformations involved in making and using metals, ceramics, electronic materials, plastics and composites are strikingly similar. Matters such as transformation mechanisms, defect behaviour, the thermodynamics of equilibria, diffusion, flow and fracture mechanisms, the fine structure and behaviour of interfaces, the structures of crystals and glasses and the relationship between these, the statistical mechanics of assemblies of atoms or magnetic spins, have come to illuminate not only the behaviour of the individual materials in which they were originally studied, but also the behaviour of other materials which at first sight are quite unrelated. This continual cross-linkage between materials is what has given rise to Materials Science, which has by now become a discipline in its own right as well as being a meeting place of constituent disciplines... Materials Technology (or Engineering) is the more practical counterpart of Materials Science, and its central concern is the processing of materials, which has become an immensely complex skill...."

Whether I was justified in saying that Materials Science "has by now become a discipline in its own right", is briefly discussed in the last chapter.

The most idiosyncratic of the materials families are polymers and plastics. The mutual illumination between these and the various categories of inorganic crystalline materials has been slow in coming, and this means that teaching polymer science in broad materials science departments and relating the properties of polymers to other parts of the course, has not been easy. Yet things are improving, partly because more and more leading researchers and teachers in polymer physics are converted metallurgists. One of these reformed metallurgists is Edward Kramer, now in the Materials Department at the University of California, Santa Barbara. In a message (private communication, 2000) he pointed to three links from his own experience:

(1) In a semicrystalline polymer, the crystals are embedded in a matrix of amorphous polymer whose properties depend on the ambient temperature relative to its glass transition temperature. Thus, the overall elastic properties of the semicrystalline polymer can be predicted by treating the polymer as a composite material

with stiff crystals embedded in a more compliant amorphous matrix, and such models can even be used to predict the linear viscoelastic properties.

(2) Thermodynamics and kinetics of phase separation of polymer mixtures have benefited greatly from theories of spinodal decomposition and of classical nucleation. In fact, the best documented tests of the theory of spinodal decomposition have been performed on polymer mixtures.

(3) A third topic is the mutual diffusion of different macromolecules in the melt. Here, the original formulation of the interdiffusion problem in metals proved very useful even though the mechanisms involved are utterly different. When a layer of polymer A with a low molecular weight diffuses into a layer of the same polymer with high molecular weight, markers placed at the original interface move towards the low-molecular-weight side, just as in Kirkendall's classical experiments with metals (Section 4.2.2). The viscous bulk flow that drives this marker displacement is equivalent to the vacancy flux in metals.

I shall be wholly convinced of the beneficial conceptual synergy between polymers and other classes of materials when polymer scientists begin to make more extensive use of phase diagrams.

In earlier chapters, especially Chapters 2 and 3, the links of materials scientists to neighbouring concerns such as solid-state physics, solid-state chemistry, mineralogy, geophysics, colloid science and mechanics have been considered, and need not be repeated here. *Suffice it to say that materials scientists and engineers have proved themselves to be very open to the broader world of science.* A good proof of this is the experience of the Research Council in Britain that distributes public funds for research in the physical sciences. It turns out that the committee which judges claims against the funds provided for materials science and engineering (a committee composed mainly of practising materials scientists) awards many grants to departments of physics, chemistry and engineering as well as to mainline MSE departments, whereas the corresponding committees focused on those other disciplines scarcely ever award funds to MSE departments.

14.2. PROFESSIONAL SOCIETIES AND THEIR EVOLUTION

The plethora of professional societies now linked to MSE can be divided into three categories – old metallurgical societies, either unregenerate or converted to broader concerns; specialised societies, concerned with other particular categories of materials or functions; and societies devoted to MSE from the time of their foundation. Beyond this, there are some federations, umbrella organisations that link a number of societies.

All the societies organise professional meetings, and often publish the proceedings in their own journals; many of the larger societies publish multiple journals. Most societies also publish a range of professional books.

14.2.1 Metallurgical and ex-metallurgical societies

There have long been a number of renowned national societies devoted to metals and alloys, some of them more than a century old. They include (to cite just a few examples, using early – not necessarily original – names) the Metallurgical Society of the American Institute of Mining, Metallurgical and Petroleum Engineers, The American Society for Metals, the Institute of Metals in London, the Deutsche Gesellschaft für Metallkunde, the Société Française de Métallurgie, the Indian Institute of Metals, the Japan Institute of Metals. Most of these have now changed their names because, at various times, they have sought to broaden their remit from metals to materials; the Indian and Japanese bodies have not hitherto changed their names. Some bodies have simply resolved to become broader; one has become simply TMS (which represents The Minerals, Metals and Materials Society), another, ASM International. Other societies have broadened by merging with other preexisting societies: thus the Institute of Metals in London first became the Metals Society, which merged with the Iron and Steel Institute to become the Institute of Metals once again, and eventually merged with other societies concerned with ceramics, polymers and rubber to become the Institute of Materials.

The journals published by the various societies have mostly undergone repeated changes of name. Thus, the old *Journal of the Institute of Metals* first split into *Metal Science* and *Materials Technology* and finally reunited as *Materials Science and Technology*. TMS and ASM International joined forces to publish *Metals Transactions*, which recently turned into *Metallurgical and Materials Transactions*; this journal replaced two earlier ones published separately by the two societies, each of these having changed names repeatedly. The German journal published by the Deutsche Gesellschaft für Metallkunde (now the D.G. für Materialkunde, DGM) was and remains the *Zeitschrift für Metallkunde*; most of the papers remain metallurgical and most of them are now in English. (The history of the DGM, "in the mirror of the Zeitschrift für Metallkunde", is interestingly summarized in an anniversary volume, DGM 1994.) The French society has replaced 'metals' with 'materials' in its name, and likewise incorporated the word in the rather lengthy title of its own journal (*Revue de Métallurgie: Science et Génie des Matériaux*). These many name changes must be a librarian's nightmare.

The underlying idea fueling the many changes of names of journals is that by changing the name, societies can bring about a broadening of content. By and large this has not happened, and the journals have remained obstinately metallurgical in character, because when a journal is first published, it quickly acquires a firm identity in the minds of its readers and of those who submit papers to it, and a change of name does not modify this identity. In my view, only a very resolute and proactive editor, well connected through his own scientific work to the scientific community, and with clear authority over his journal, has any hope of gradually bringing about a genuine transformation in the nature of an existing, well-established journal. The alternative, of course, is to start completely new journals, some independent of societies; this alternative strategy is discussed in Section 14.3.

In Europe, a Federation of Materials Societies, FEMS, was established in 1987; it links 19 societies in 17 countries (website: http://www.fems.org). It plays a role in setting up Europe-wide conferences on materials, keeps national societies informed of each other's doings, and seeks to avert timetable conflicts. Further federations feature in the next section.

14.2.2 Other specialised societies

Numerous societies are devoted to ceramics, to glass or to both jointly. The American Ceramic Society is the senior body; the European Ceramic Society is an interesting example of a single body covering a wide but still restricted geographical area. Societies covering polymers (and elastomers sometimes treated as a separate group) are multifarious, both nationally and internationally. Still other specialisms, such as composite materials, carbon and diamond are covered by commercial journals rather than by specialised societies, but even where there is no society to organise conferences in a field, yet independent and self-perpetuating groups of experts arrange such conferences without society support. Semiconductor devices and integrated circuits are mostly covered by societies closely linked to the electrical engineering profession. There are a number of societies, such as the Royal Microscopical Society in Britain, which focus on aspects of materials characterization. Any attempt to list the many specialised professional bodies would be unproductive.

14.2.3 Materials societies **ab initio**

The first organization to carry the name of materials science was a British club, the Materials Science Club, founded by a group of materials-oriented British chemical engineers in 1963. This group organised broad meetings on topics such as 'materials science in relation to design' and 'biomechanics', and published some of the contributions in its own quarterly *Bulletin*. The Club brought together a very wide range of some hundreds of scientists and engineers from universities, industry and government laboratories, including a proportion of foreign members, awarded medals, and published almost 100 issues of its *Bulletin* before difficulties in organising its affairs without any paid staff eventually brought about its absorption, in the late 1980s, by the Institute of Metals in London, and thereby its extinction. Only one complete set of the *Bulletin* survives, in the library of the City University in London. While it lasted, it was a very lively organization.

Undoubtedly, the key organization created to foster the new concepts of interdisciplinary research on materials is the Materials Research Society, MRS, founded in the US in 1973, after 7 years of exhaustive discussions. It is to be particularly noted that its name carries the words 'Materials Research', not 'Materials Science'. 'Materials Research' avoids specifying which kinds of scientists and engineers should be involved in the society; all that is required that their work should contribute to an understanding and improvement of materials. According to illuminating essays (Roy and Gatos 1993) by two of the founders of the MRS, Rustum Roy and Harry Gatos (whom we have met in Section 10.4.1), from the start the society was to focus on research involving cooperation between different disciplines, of which MSE was to be just one – albeit a vital one. Gatos is forthright in his essay: "The founding and operation of MRS was the culmination of my ten years of frustrated effort in searching for a professional home (old, renovated or new) for the young, homeless materials science. The leaders of the existing materials societies strenuously resisted accepting that materials science existed outside the materials they dealt with, be they metals, ceramics, or polymers. The founders of MRS were just a small but 'driven' minority..." Certainly my own experience of starting Britain's first university department of materials science in 1965 confirms what Gatos (who was at MIT) says about professional societies at that time; when I first attended a meeting of the MRS in 1976, I realised that I had found my primary intellectual home, inchoate though it was in that year. The MRS took some years to reach its first 1000 members, but after that grew rapidly.

There was a further consideration in the minds of the founders, though that has been kept rather quiet in public. In the early 1970s, physicists and chemists working in American industry, especially the many working on aspects of materials, were not made welcome in their professional physics and chemistry societies, which were inclined to ignore industrial concerns. These two groups played a substantial part in bringing the MRS to life; it must also be said immediately that enlightened figures in industry, especially William O. Baker, director of research at Bell Telephone Laboratories, from an early stage supported MRS by word and deed. MRS from the beginning welcomed industrial scientists and topics of close concern to industry. It is thus natural that today, as many as 25% of the ≈12,500 members of MRS (in more than 60 countries) are in industry (as against 63% in academe and 12% in government laboratories) (Rao 2000).

Roy and Gatos, as also Phillips (1995) in her even more recent snapshot of the MRS, all emphasise two features of the society: the major role of volunteer activity by members in taking scientific decisions and making the society work (in its early years, it had no paid staff), and the invention of the principle of simultaneous symposia, organized by members, each on a well-defined, limited topic, that constitutes the main business of the society's annual meetings, a practice, as Roy points out, "now copied almost universally by most disciplinary societies." Several hundred volumes of proceedings of these symposia have been published by 2000. The MRS now has a large, paid headquarters staff, essential for what has become a large and variegated organization.

In addition to the symposium proceedings, MRS publishes a monthly *MRS Bulletin*, and in 1986 it founded an archival research journal, *Journal of Materials Research* (*JMR*), and both are going strong. I have had many occasions in this book to cite expository articles in the *Bulletin*, in particular. The *JMR* is run in an unusual way, typical of the MRS: each submitted paper is sent to one of a panel of principal editors (chosen periodically by the society's council) and he/she reports on the paper to the Editor-in-Chief, who alone communicates with authors. I was one of the first batch of principal editors, and found that this system worked well. An essay on the genesis and principles of this journal, three years afterwards, was published by Kaufmann (1988). *JMR* has only one Achilles' heel: as Roy (1993) pointed out, "the MRS has not been able to involve the polymer community to a major extent; less than 5% of the *JMR* is (in 1993) devoted to polymers." This is a lasting problem for all who seek to foster a broadly based discipline of MSE. However, *JMR* is publishing an increasing proportion of papers on the broad theme of materials processing, and this is a particularly useful service.

Once it was well-established, and mindful of its many foreign members, the MRS encouraged the progressive creation of local MRSs in a number of countries. There are now 10 of these, in Australia, China, Mexico, Argentina, India, Japan, South Korea, Russia, Taiwan and Europe (embodying various European countries, and domiciled in France). Some are more active than others; in particular, the Indian body, MRS-I, publishes its own successful research periodical, *Bulletin of Materials Science*, and the Chinese MRS has organized a succession of major international conferences. Overarching these societies is the International Union of Materials Research Societies; the original MRS has helped a great deal in setting up this federal supervisory body, but in no sense does it dominate it. One example of the help this federation gives to constituent bodies is a major MSE conference held in Bangalore, India, in 1998 (proceedings, IUMRS-ICA 98 1999).

In Japan, the Japan Federation of Materials acts as an umbrella organisation for 18 Japanese materials societies, and very recently, in 2000, it has co-sponsored a new English-language Japanese journal, *Science and Technology of Advanced Materials*, with (among other aims) the laudable editorial objective of "concise presentations, so that interested readers can read an issue from cover to cover."

One primary aim of the MRS, to achieve a breakdown of interdisciplinary barriers, has been well achieved, according to one of the prime godfathers of materials science, the American Frederick Seitz (Fig. 3.19, Chapter 3). In a book primarily devoted to Italian solid-state physics (Seitz 1988), he remarks: "I might say a few words about the 55 odd years in which I have been associated with solid-state physics or, as it is sometimes called in the US, solid-state science, or condensed matter physics or materials science. When I entered the field as a graduate student in the early 1930s the overall field was strongly compartmentalised into three divisions which had relatively little interaction... One division was related to work in the field of metallurgy and ceramics... The second division related to research on materials for electrical engineering and electronics,... The third division related to the investigations of what might be called the fundamentalist scientists." Of these three divisions, Seitz says: "While these divisions still exist, the flow of information between them is now much greater than it was and the research groups in each have many common bonds, mainly because of the application of solid-state physics." This is a robust physicist's view of the broadening of materials research.

Of course, many other professional societies have played their part in this successful reaching out between specialisms. As outlined above, the big metallurgical societies have broadened resolutely, and the American Physical Society and American Chemical Society are now much more hospitable to their members in industry than they apparently were 30 years ago.

14.3. JOURNALS, TEXTS AND REFERENCE WORKS

There is now an immense range of scientific journals, broad, narrow and in-between, to serve the great range of materials. The journals published by the many professional societies have encountered increasing competition from the many published by commercial publishers, but those, in turn, are now under severe pressure because of a growing librarians' revolt against subscription prices that rise much faster than general inflation.

14.3.1 Broad-spectrum journals

One classification is of special importance: there is a small minority of materials journals that can be described as *broad-spectrum*, compared with a much larger number which are specialised to a greater or lesser degree. Probably the first broad-spectrum journal was *Journal of Materials Science*, *JMS*, launched by a commercial publisher in 1966. I was the first chairman of editors, so had a major role in forming policy. My insistence was that there should be several editors with complementary fields of expertise and independent powers of decision over submitted papers, and I encouraged those editors to be proactive (to use a current jargon-word) and seek out key papers on novel topics. This worked well, and the publication of such key papers then encouraged other authors in the same field to steer their papers to *JMS*. The 1969 paper from which Fig. 6.6 (Chapter 6) was reproduced was an example of this successful policy. Since the journal was broad-spectrum *from the beginning* (including, incidentally, polymer physics) that was how it has always been perceived and it has not become specialised, even when the 6 editors had to be replaced by one editor after some years (because of my enhanced academic duties in 1973 that deprived me of time to edit). However, there have been several spin-off mini-journals, including one devoted to the new editor's specialism, biomedical engineering. *JMS* has also always been very international.

Another journal, *Materials Science and Engineering* (*MSE*), was started by another commercial publisher at about the same time as *JMS*. This had only one editor, a metallurgist, from the start, and so in spite of its stated objectives, it remained almost wholly metallurgical for many years. When eventually it became broader under a new editor, it was split into several independent journals with distinct editorial boards, each of them relatively broad-spectrum – in particular, one devoted to functional materials, and another to biomimetics. The main *MSE* remained in being, and has remained largely metallurgical after 35 years.

The MRS archival journal, *Journal of Materials Research*, already mentioned, is another broad-spectrum journal that has worked well, except for its limited polymer content. Here again, the principle of multiple editorship seems to have been an important component of success.

Some older journals, such as *Journal of Physics and Chemistry of Solids*, which has been published for some 60 years and now focuses to some degree on functional materials, have long been broad-spectrum. Others have a broad-spectrum name but in fact are relatively narrowly focused: an example is *Materials Research Bulletin*, which in fact is concerned mostly with the chemistry of inorganic materials. Its subtitle is *an international journal reporting research on the synthesis, structure and properties of materials*. (This journal now has a supplement entitled *Crystal Engineering*.) Likewise, an English-language journal simply called *Advanced Materials* began publication 10 years ago in Germany, and is highly successful; in spite of its comprehensive title, it is wholly focused on materials chemistry, especially processing. In recent years, the archetype of broad spectrum, *Nature*, has begun to pay special attention to papers on materials processing, self-assembly techniques in particular, as the many references to that journal in Chapter 11 testify.

In Russia, after many years of a successful but purely metallurgical journal entitled *Fizika Metallov i Metallovedenie* (the last word representing 'knowledge of materials' and not, as I had supposed, 'metallography' (Rabkin 2000)), a group of influential materials scientists in 1997 started a journal entitled *Materialovedenie*, which word I believe to be the best current Russian form of 'materials science'. In spite of the editors' best efforts, the journal is finding it difficult to break away from a metallurgical focus.

In Japan, as recorded above, a new journal called *Science and Technology of Advanced Materials* has just begun publication.

An interesting, broad-spectrum journal founded in 1997 by Roy is *Materials Research Innovations*; one of its objectives is to bypass normal methods of editorial scrutiny; submitting authors who have published a sufficient number of papers in other, peer-reviewed, journals are assumed, in effect, to have reviewed themselves.

A number of journals devoted wholly to review articles, shading from metallurgy to genuine materials science, are now appearing; the grandfather of this group is *Progress in Materials Science* (which began in 1949 as *Progress in Metal Physics*). Another excellent example is *Materials Science and Engineering – Reports: A Review Journal*.

14.3.2 The birth of Acta Metallurgica

The journal whose genesis is to be described here is of extreme importance in the history of modern physical metallurgy and, later, materials science. Its birth in 1953 coincided with the high point of the 'quantitative revolution' portrayed in Chapter 5, and preceded by a few years the beginning of materials science. It transformed the metallurgical researcher's perception of the discipline and it clearly contributed to the currents of thought that first brought materials science into being in 1958.

Acta Metallurgica owed its birth to a resolute metallurgist, Herbert Hollomon, whom we met in Section 1.1.2 in his capacity as leader of materials research at the General Electric Corporate R&D Center in New York State. According to a history of the journal (Hibbard 1988), an update thereto (Fullman 1996) and private information from Seitz (2000), Hollomon perceived soon after World War 2 that publications from a new post-war surge of research were widely scattered throughout the physical, chemical and metallurgical literature and that there was a "need for a unifying journal in which the fruits of such research could be gathered more effectively." A number of eminent researchers, including among others Frederick Seitz, Harvey Brooks (the founding editor of *Journal of Physics and Chemistry of Solids*), Cyril Stanley Smith (see Section 14.4.1) and Bruce Chalmers, joined in discussions that led, in 1951, to an approach to the American Society of Metals which then offered generous financial support; in this the ASM was later joined by the American Institute of Mining, Metallurgical and Petroleum Engineers. During the next year, a board of governors chaired by Smith was created, and appointed Bruce Chalmers, then a professor in Toronto, Canada (see Section 9.1.1) to be editor. Hollomon was secretary/treasurer of the board of governors.

Acta Metallurgica began publication in the spring of 1953 and at once created a huge impact in the profession with its many rigorous, quantitative papers, long and short. The journal's standards were very high from the beginning, and aspects of physics (such as for instance nuclear magnetic resonance) found their place in the journal from the first volume. Cyril Smith, in his preface to the first issue, memorably remarked: "Now, metallurgy is too broad to be encompassed by a single human mind: it is essential to enlist the interest of the 'pure' scientists, and to increase the number of metallurgists whose connections with production and managerial problems are partially sacrificed in order that they may be more concerned with physics and physical chemistry as a framework for useful metallurgical advance."

By 1967, the flood of short papers had become so great that a separate journal, *Scripta Metallurgica*, was hived off. These Latin titles were intended to symbolise the international character of the journal. Chalmers edited the journal until 1974, when Michael Ashby took over the reins which he held until 1995; at that point a more collegiate editorial structure was instituted. In 1990, the adjective '*metallurgica*' was supplemented by '*materialia*', and in 1996 the journals simply became *Acta materialia* and *Scripta materialia* (some classicist seems to have advised the board of governors, at a late stage, that lower case letters are de rigueur in Latin!)

Acta Metallurgica was unique among journals in having from the beginning a completely independent board of governors which is the formal owner, permanently guaranteed financially by the two leading American metallurgical societies. The initially contracted publisher in Toronto proved to have difficulty in sustaining the printing effort, and when it seemed that the project might be stillborn, Seitz (then chairman of the governing board of the American Institute of Physics) brought in the publishing facilities of that Institute to rescue the situation; much effort was involved in the rescue. By that time, Chalmers had moved to Harvard. However, in 1955 Hollomon met Robert Maxwell, proprietor of Pergamon Press, on an airplane; they took to each other (both were forceful characters to a degree) and Hollomon, who seems to have had quasi-dictatorial powers over the board of governors of *Acta Metallurgica*, insisted that Pergamon Press should take over publication of the journal; it has published it (and its temporary sister publications... like *Materials and Society*) since 1955. However, Pergamon Press has never owned the copyright or the journal itself, and policy decisions have always been taken by the board of governors with input from a very international roster of advisers.

In recent years, under the leadership of a coordinating editor, Subra Suresh, *Acta Materialia* and its letter journal have sought energetically to broaden the remit of the journals, with some success but also some difficulties. In January 2000, Suresh edited a fine 'millenium issue', entitled *Materials science and engineering: current status and future directions*; it included 21 overviews, including excellent treatments of polymers.

14.3.3 Specialised journals

Scientific journals devoted to particular categories of materials, or procedures, become ever more numerous. Some are national, others continental or international in scope; some are highly specific, others somewhere between broad and narrow spectrum; some publish in English or another language only, others accept papers in several languages. All I can usefully do here is to cite a few examples.

An example of a journal hovering between broad and narrow spectrum is *Journal of Alloys and Compounds*, subtitled "an interdiciplinary journal of materials science and solid-state chemistry and physics." One which is more restrictively focused is *Journal of Nuclear Materials* (which I edited for its first 25 years). Ceramics has a range of journals, of which the most substantial is *Journal of the American Ceramic Society*. *Ceramics International* is an example of an international journal in the field, while *Journal of the European Ceramic Society* is a rather unusual instance of a periodical with a continental remit. More specialised journals include *Solid State Ionics: Diffusion and Reactions*, and a new *Journal of Electroceramics*, started in 1997.

Polymer journals are very plentiful and most of them are relatively broad in coverage. Examples – *Polymer* (*the international journal for the science and technology of polymers*), *Progress in Polymer Science* and *New Polymeric Materials*. To repeat a statement made in Chapter 2: "As late as 1960, only four journals were devoted exclusively to polymers – two in English, one in German and one in Russian. Now, however, the field is saturated: a survey in 1994 came up with 57 journal titles devoted to polymers that could be found in the Science Citation Index, and this does not include minor journals that were not cited."

Other examples of specialised journals include *Composites Science and Technology*; a broad journal called *Carbon* and a more specific one, *Diamond and Related Materials*; and *Biomaterials* (incorporating *Clinical Materials*). I have already mentioned the new *Crystal Engineering*, which joins such journals as *Crystal Research and Technology* and in turn was joined in 2001 by *Crystal Growth and Design*. Beyond that, there are the several forms of the classic journal *Acta Crystallographica* (which may have been the first to adopt a Latin title). A whole series of new journals cover computer modelling and simulation of materials: *Computational Materials Science* is one, *Modelling and Simulation in Materials Science and Engineering* is another.

A large group of journals covers various aspects of characterization, including electron microscopy. *Micron* and *Ultramicroscopy* are two of these, *Materials Characterization* (published in association with the International Metallographic Society) is another.

Materials chemistry is now served by a whole range of journals, ranging from the venerable *Journal of Solid-State Chemistry* and *Materials Research Bulletin* (already mentioned) to *Materials Chemistry and Physics* (which, interestingly, now incorporates *The International Journal of the Chinese Society for Materials Science...* which appears to be distinct from the Chinese MRS) and *Journal of Materials Chemistry* (published by the RSC in London) – also *Chemistry of Materials*, published by the ACS. In France, *Annales de Chimie: Science des Matériaux* is an offshoot of a journal originally founded by Lavoisier in 1789 (shortly before he lost his head). *Journal of Materials Synthesis and Processing* is an interesting periodical with somewhat narrower focus.

In this listing of examples, I have excluded straight metallurgical journals and the many devoted to solid-state physics, such as the venerable *Philosophical Magazine* and *Physical Review B*.

14.3.4 Textbooks and reference works

One of the defining features of a new discipline is the publication of textbooks setting out its essentials. In Section 2.1.1, devoted to the emergence of physical chemistry, I pointed out that the first textbook of physical chemistry was not published until 1940, more than half a century after the foundation of the field. Materials science has been better served. In what follows, I propose to omit entirely all textbooks devoted to straight physical metallurgy, of which there have been dozens, say little about straight physics texts, and focus on genuine MSE texts.

As we saw in Chapter 3, the founding text of modern materials science was Frederick Seitz's *The Modern Theory of Solids* (1940); an updated version of this, also very influential in its day, was Charles Wert and Robb Thomson's *Physics of Solids* (1964). Alan Cottrell's *Theoretical Structural Metallurgy* appeared in 1948 (see Chapter 5); although devoted to metals, this book was in many ways a true precursor of materials science texts. Richard Weiss brought out *Solid State Physics for Metallurgists* in 1963. Several books such as *Properties of Matter* (1970), by Mendoza and Flowers, were on the borders of physics and materials science. Another key 'precursor' book, still cited today, was Darken and Gurry's book, *Physical Chemistry of Metals* (1953), followed by Swalin's *Thermodynamics of Solids*.

However, the first text specifically for students of materials science was Lawrence van Vleck's *Elements of Materials Science: An Introductory Text for Engineering Students* (1959), which was very widely used. It appeared only a year after the initiatives at Northwestern University which gave birth to MSE (Section 1.1.1). In 1970, he published *Materials Science for Engineers*. Later, in 1973, the same author brought out *A Textbook of Materials Technology*; in his preface to this, van Vlack says that it was prepared "for those initial courses in materials which need the problem-solving approach of the technologist and the engineer, but which must fit into curricula designed for those who have a minimal background in the sciences." Thus its approach was very different from Morris Fine's book, mentioned next.

In 1964, two competing series of slender volumes appeared: one, the 'Macmillan Series in Materials Science', came from Northwestern: Morris Fine wrote a fine account of *Phase Transformations in Condensed Systems*, accompanied by Marvin Wayman's *Introduction to the Crystallography of Martensite Transformations* and by *Elementary Dislocation Theory*, written by Johannes and Julia Weertman. The second series, edited at MIT by John Wulff, was entitled 'The Structure and Properties of Materials', and included slim volumes on *Structure*, *Thermodynamics of Structure*, *Mechanical Behaviour* and *Electronic Properties*.

From the early 1970s onwards, more substantial texts began to appear, notably Arthur Ruoff's *An Introduction to Materials Science* (1972), a book of 700 pages. This was followed by *The Principles of Engineering Materials* (1973) by Craig Barrett, William Nix and Alan Tetelman, then *Metals, Ceramics and Polymers* (1974), 640 pages, by Oliver Wyatt and David Dew-Hughes (the first book, after Cottrell's, by British authors), and then another British book, *Structure and Properties of Engineering Materials* (1977) by Bryan Harris and Anthony Bunsell. In Germany, Erhard Hornbogen brought out *Werkstoffe* (1973). In the Ukraine (while the Soviet Union still existed) an anonymous editor brought out a multiauthor volume (in Russian) entitled *Fizicheskoe Materialovedenie v SSSR* (1986); this is probably the only such book ever to focus on research in one country. In 1982, I.S. Miroshnichenko brought out a specialised book on quenching (of alloys) from the melt. Very recently, Bernhard Ilschner in Lausanne has masterminded a series of texts in materials science in the French language.

A fresh start has been made by Samuel Allen and Edwin Thomas of MIT, with *The Structure of Materials* (1998), the first of a new MIT series on materials. The authors say that "our text looks at one aspect of our field, the structure of materials, and attempts to define and present it in a generic, 'materials catholic' way." They have succeeded, better than others, in integrating some crucial ideas concerning polymers into mainline materials science.

A number of somewhat more specialised texts also began to appear, such as Anderson and Leaver's *Materials Science* (1969); in spite of its broad title, this book by two members of the Electrical Engineering Department at Imperial College, London, was wholly devoted to electrical and magnetic (functional) materials. So was *Electronic and Magnetic Behaviour of Materials* (1967) by Allen Nussbaum of the University of Minnesota.

A good example of a book aimed specifically at processes is Alexander and Brewer's *Manufacturing Properties of Materials* (1963). More recently, there have been some fine texts aimed directly at developing for fledgling engineers a systematic approach for selecting materials during the design process: *Engineering Materials – an Introduction to their Properties and Applications* (1980), by Ashby and Jones, is probably the best example.

There have also been some excellent books and collections of articles written at a popular level. The master of this difficult art was James (J.E.) Gordon, who brought out two immensely successful titles, *The New Science of Strong Materials, or Why You Don't Fall Through the Floor* (1968) and *Structures, or Why Things Don't Fall Down* (1978). The magazine *Scientific American* consecrated the issue of September 1967 entirely to a number of surveys of materials, from a very wide range of perspectives; the lead article was by Cyril Stanley Smith. These articles also came out as a book, *Materials*, published by Freeman. In October 1986, another issue of the same periodical was devoted to materials for economic growth. In 1980, the great French physicist André Guinier (the discoverer of zones in precipitation-hardened light alloys), brought out *La Structure de la Matière, du Ciel Bleu à la Matière Plastique*; this was later translated into English. I have myself for many years contributed 1000-word articles to *Nature* on many aspects of materials science: a selection of 100 of these appeared in 1992 under the title *Artifice and Artefacts*.

A valuable source of up-to-date reviews of many aspects of MSE is a series of books, *Annual Reviews of Materials Science*, published for the last 30 years. There has been one extensive series of high-level multiauthor treatments right across the entire spectrum of MSE, in the form of 25 books collectively entitled *Materials Science and Technology: A Comprehensive Treatment* (1991–2000), masterminded by Peter Haasen, Edward Kramer and myself. There have also been three encyclopedias, *the Encyclopedia of Materials Science and Engineering* (1986), the *Encyclopedia of Advanced Materials* (1994) and the *Encyclopedia of Materials* (2001), which last has appeared in both printed and on-line versions and will receive annual updates.

14.4. MATERIALS SCIENCE IN PARTICULAR PLACES

Recently, at an international conference, during the 'afternoon off' when we were all ambling in the sunshine, a young Algerian student asked me for a 'word of wisdom'. What elderly scholar can resist such a dewy-eyed approach from youth? So I reflected for a moment and then told him: "Remember that there is not really such thing as Algerian science... or British or American science. There is just science, a worldwide collective endeavour. The thing that is invariant is the belief in the importance of a form of internationalism that really works, a pursuit of truth that unites mankind." This last sentence is a formulation that I owe to my wife.

What I said to the young man was both true and untrue. It is quite true that working with, or at least communicating with, one's colleagues worldwide is one of the things that most makes a life in science worth while. Yet what one can do in a particular place depends on the resources and stimulus available, which in turn depend on the traditions and economy of that place. For instance, the traditions of (say) a Middle Eastern country may predispose scientists (and even engineers) there to focus on theoretical work at the expense of experiment. So in that limited sense, there is interest in saying something about how materials science and engineering have developed in different places, and to try to draw some conclusions. That is my objective in this section. I have picked people and institutions on the basis of personal acquaintance in years past, and that is why there is a certain metallurgical bias in my choices, since my personal research was on metals. I have outlined *particular* institutions in the USA, Japan, Australia (with an aside on Germany), Argentina and Russia, and tried to paint brief portraits of the people that brought them into being. I have not attempted the hopeless task of painting a complete portrait of those countries.

Those countries apart, if there were much more space available I could outline research institutions for materials science in the many European countries that possess them, in India, China and Korea, in Canada, Brazil, Israel. The fact that I do not implies no disrespect for the many fine experts in those lands.

14.4.1 Cyril Smith and the Institute for the Study of Metals, Chicago

A number of American research institutions and the people who shaped them have already featured in this book: the creation of the Materials Research Laboratories; Robert Mehl's influence on the Naval Research Laboratory and on Carnegie Institute of Technology; Hollomon's influence on the GE laboratory; Seitz's influence on the University of Illinois (and numerous other places); Carothers and Flory at the Dupont laboratory; the triumvirate who invented the transistor and the atmosphere at Bell Laboratories that made this feat possible; Stookey, glass-ceramics and the Corning Glass laboratory. I would like now to round off this list with an account of a most impressive laboratory that came to grief, and the man who shaped it.

Cyril Stanley Smith (1903–1992) (Fig. 14.2) was a British-born metallurgist who studied at Birmingham University and then emigrated to the United States as a young man, took a doctorate at MIT, and spent 16 years as a successful researcher

Figure 14.2. Portrait of Cyril Stanley Smith in old age (courtesy of MIT museum).

on alloys in an industrial copper-and-brass company; he obtained numerous patents. He became well known for the originality and clarity of his researches, and in 1943 Robert Oppenheimer recruited him to be joint head of the metallurgical effort in the bomb project at Los Alamos. When the War ended in the summer of 1945, he agreed to an invitation from the University of Chicago (which had a highly active president, Robert Hutchings) to create there a novel kind of laboratory devoted to the study of metals in particular, and the solid state more generally. In 1946, the Institute for the Study of Metals opened its doors on the Chicago campus in the same building where in 1942 the world's first nuclear reactor had gone critical. (It is ironic that this earlier project at the time was called 'The Metallurgical Laboratory of the Manhattan District' with the aim of totally confusing anybody who might have been inquisitive.) An account of the first 15 years of the Institute, by one of its members, has recently appeared (Kleppa 1997).

In April 1946, a few months before the Institute began operation, Smith made public a memorandum detailing the principles on which it was to be founded. (The memorandum is reprinted in Kleppa's paper, and might be described as an elaboration of the ideas concisely set out 7 years later in Smith's preface to the first issue of *Acta Metallurgica*, from which some words are quoted in Section 14.3.2) Indeed, the creation of the Institute and later of *Acta Metallurgica* were two sides of one coin. In his memorandum, Smith saw physicists as the masters of theoretical work on metals, physical chemists as students of reactions and of the associated thermodynamics, while metallurgists would undertake research on matters like diffusion, phase transformations, grain growth, and "similar fields in which a phenomenological approach must precede or accompany the strictly mathematical". He also indicated, fatefully, that "the Institute will maintain close connections with the instructional activities of the university, but it is not intended to establish a separate Department of Metallurgy, and consequently, no degrees in metallurgy will be awarded."

Cyril Smith succeeded in attracting some very distinguished researchers at the beginning, including Charles Barrett (who had worked with Mehl in Pittsburgh), Clarence Zener, Norman Nachtrieb, the eminent crystallographer William Zachariasen, Andrew Lawson, Joseph Burke, Earl Long, the Chinese T'ing-Sui Kê... to mention only a few of the metallurgists, ceramists, physicists and chemists whom Smith had recruited (partly drawing on his acquaintances at Los Alamos). Smith also secured a large group of industrial sponsors, drawing on his industrial past. The Institute published a series of quarterly reports, distributed to the sponsors and some other favoured recipients; these reports in the early years contained entire papers which later appeared in journals, especially *Physical Review* (*Acta Metallurgica* not yet being in existence). Even most of the text of Zener's short but extremely influential book, *Elasticity and Anelasticity of Metals*, published by the University of Chicago Press in 1948, first saw the light of day in a quarterly report. Many topics were unusual, for instance Barrett's work on low-temperature phase transformations and Nachtrieb's on diffusion under hydrostatic pressure (which delivered insights into diffusion mechanisms). The Institute quickly came to be perceived as the leading fundamental research laboratory devoted to metals, and many visitors came; one was Brian Pippard, who in 1955–1956 performed there his famous work on the shape of the Fermi surface in copper (Section 3.1).

Smith himself stimulated many researchers but, though he wrote a celebrated paper on the evolution of microstructure, did not take any graduate students, and so he did not perhaps initially perceive the implications of the fact that large numbers of doctoral students came from the university's physics and chemistry departments to work with some of the permanent Institute staff... but there were no metallurgically trained students to draw on. Some of the Institute staff became closely involved with the physics or chemistry departments, and one even became chairman of the physics department. A consequence of this situation was that Smith could not attract further metallurgists to join the Institute, and junior metallurgists who came for short attachments found that they did not want to stay permanently, even when offered tempting posts. Smith's initial decision not to push for the creation of a metallurgy department proved to be the occasion of the Institute's downfall in the end, because the metallurgists had no sense of belonging to the university as a whole.

In 1955, Smith took a year's sabbatical to pursue his interests in metallurgical history (see, for instance, Section 3.1.2) which led in 1960 to the publication of his *A History of Metallography*. Earl Long became director, but resigned when in 1961 the Institute in effect was taken over by the physicists and chemists and its name was changed to the James Franck Institute (after a German émigré physicist), still its name today. It was a classic organisational coup, and nothing was said about it in the next quarterly report. Interest in metals lapsed almost completely, though Charles Barrett remained for a time. Kleppa, the author of the valedictory article cited above, was the most persistent of the early staff members, and carved out a distinguished place for himself as an expert on experimental thermochemistry of alloys (see an autobiographical paper, Kleppa 1994).

Smith resigned in 1961 and returned to his alma mater, MIT, where he developed his renowned work on the history of metallurgy, drawing on an enormous collection of ancient texts which he had begun to form in the 1930s. It would be fair to say that his courageous conception at Chicago eventually failed, and turned into something entirely different with his departure, because there was no academic home for the metallurgists on the Institute staff and the lack of such a home impeded recruitment and retention of staff. Scientists, like all other people, need a sense of belonging. In the various National Laboratories in America where so much distinguished research on materials goes on today, there is no such problem, but universities are different.

14.4.2 Kotaro Honda and materials research in Japan

When, in 1867, the repressive shogun was overthrown, the Meiji (Imperial) Restoration took place and Japan was at last thrown open to the world, the Japanese government soon recognised that Japan had a lot of catching up to do with respect to science and engineering. At once, a number of foreign professors were recruited to teach at Japanese universities, especially from Germany, Britain, France and America. One of those who came was Alfred Ewing, the many-faceted magnetician and engineer whom we met in Chapter 3. He lectured at the physics department at the Imperial University of Tokyo, 1878–1883 and proved effective in instilling an interest in magnetism among the students there. The variegated ways in which the Japanese government located and persuaded such foreign experts to help Japan, and the national differences in the behavior of such experts, are interestingly examined in a book about the 'formation of science' in Japan (Bartholomew 1987).

Honda (1870–1954) was a farmer's son. He had a difficult youth, looked down on by his father and suffering from low self-esteem. His brother talked him out of adopting agriculture as a profession and eventually he went to Tokyo to study physics, where he graduated in 1897. Clearly, Ewing's influence was still felt there, because Honda homed in on magnetism for his initial research. He stayed in Tokyo for 10 years, influenced by Hantaro Nagaoka, an excellent teacher of physics who was interested in metals and magnetostriction, and acquired a doctorate. In 1907, the Ministry of Education awarded him a travelling scholarship and he spent the next 4 years divided between Gustav Tammann in Göttingen (a metallurgist, see Fig. 3.8) and René Du Bois in Berlin (a magnetician). Fig. 14.3 shows a photograph of Honda at this time, as well as a later photograph when he had become famous in Japan. Both photographs suggest how thoroughly he had overcome the handicaps of his childhood. In these years in Europe, he studied the changes in magnetic properties of numerous elements as a function of temperature, and also the periodicity of the atomic susceptibility in a range of metals (Honda 1910). He spent a week with Ewing (who was now in Cambridge), discussing his findings, and received Ewing's praise. Like many Japanese who visited the west, Honda was much influenced by at least one of his teachers, and became as brusque and demanding with his collaborators as was Tammann, and would not brook contradiction. Honda, having overcome his own childhood inferiority, was wholly unimpressed by other people's class or status. According to contemporary records, however, he did not share Tammann's quick temper and was always imperturbable.

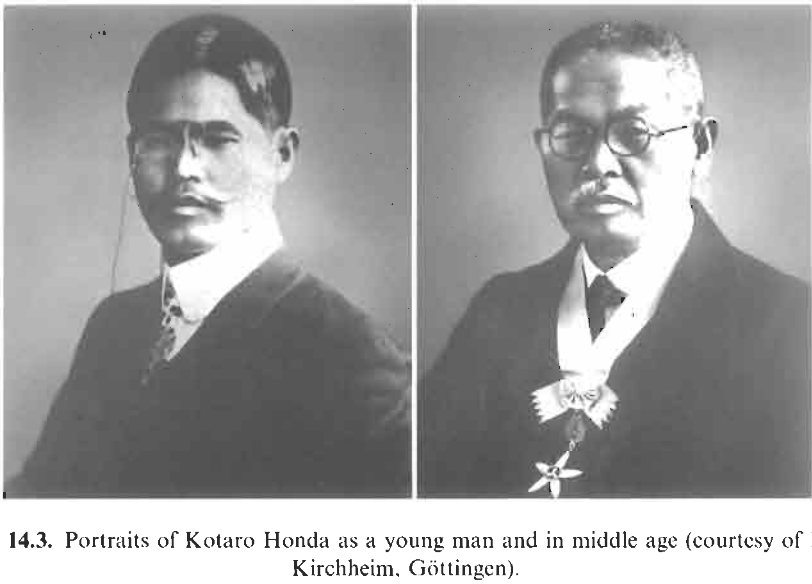

Figure 14.3. Portraits of Kotaro Honda as a young man and in middle age (courtesy of Reiner Kirchheim, Göttingen).

On his return home in 1911, Honda was appointed professor of physics at the new Tohoku Imperial University in Sendai, in the north of Japan; this institution had been established only in 1906, when the finance minister twisted the arm of an industrialist who had made himself unpopular because of pollution caused by his copper mines and extracted the necessary funds to build the new university. A provisional institute of physical and chemical research was initiated in 1916, divided into a part devoted to novel plastics and another to metals. This proved to be Honda's lifetime domain; he assembled a lively team of young physicists and chemists. In the same year, Honda invented a high-cobalt steel also containing tungsten and chromium, which had by far the highest coercivity of any permanent-magnet material then known. He called it KS steel, for K. Sumitomo, one of his sponsors, and it made Honda famous.

In 1919, after much politics (the details of which can be found in Bartholomew's book) Honda's group was inaugurated under the name of Iron and Steel Research Institute. Three years later, to broaden its terms of reference, it was rechristened the Research Institute for Iron, Steel and Other Metals (RIISOM). The Institute was wholly focused on intensive research, at all hours of the day and night; Honda was full of scientific ideas and implacable with his colleagues and students. Among many other early successes were a series of improved magnetic alloys, details of which can be found in a survey of Japanese research in magnetism (Chikazumi 1982). Honda succeeded in always maintaining an excellent balance between fundamental and applied concerns. (According to Bartholomew, "the business interests that came to support him thought his work theoretical, but academics thought it applied.") By the end of Honda's reign, Japan had moved a long way from the view expressed in a 1907 editorial, that basic researchers were "eccentrics whose work is a form of dissipation."

The prodigious research output of the Institute often first saw the light of day in the *Science Reports of the Tohoku Imperial University*, and its successors; in my younger days, I received these regularly and found them rivetting reading.

In 1931, Honda, loaded with honors, became president of the university, and the Institute was directed by a successor. The Institute expanded its space, personnel and range of interests, until in 1987, in the words of the current descriptive brochure, "it was reorganised as a countrywide collaborative research institute to meet the rapid progress in materials science and renamed Institute for Materials Research." Its institutional centre has remained in Sendai. Its constituent 31 laboratories range from very pure to very applied science, from crystal physics to irradiation studies, from low-temperature physics to solid-state chemistry under high pressure, from high-purity metals to crystal chemistry, from magnetism to solidification and casting metallurgy – to name just a few. One recent director was Tsuyoshi Masumoto, who made his name in research on metastable alloys and has very recently founded a new broad-spectrum journal, *Science and Technology of Advanced Materials*, mentioned in Section 14.3. A recent director was Hiroyasu Fujimori, another distinguished physicist and metallurgist.

Today, there are many eminent researchers on materials in Japan, alike in universities and in various national research institutes, and latterly in Tsukuba Science City – but the Tohoku Institute has always held a special place, owing to the energy, determination and organising ability of its founder and the habits of work which he instilled in his staff.

14.4.3 Walter Boas and physics of solids in Australia

In the 1930s, the world's greatest migration of scientists took place under the lash of Nazism. It has sometimes been asserted that Hitler may have lost the War because of the talent he forced to flee, and that the American development of the atomic bomb that shortened the War so drastically might have been much slower without that migration. Other, less cataclysmic, consequences also flowed from the migration, and this Section is devoted to one of them.

Walter Boas (1904–1982) (Fig. 14.4) was a German physicist of Jewish parentage. In 1922 he entered the Technische Hoschschule in Berlin to study electrical engineering, but two years later he switched to physics because "I wanted a sounder grounding in fundamentals and disliked the large amounts of design work..." These words come from Boas's personal record deposited with the Australian Academy of Sciences in 1973 (with a 1979 addendum). In Berlin, Boas was stimulated by the great physicists who crowded that city, and lived through the heroic days of early wave mechanics. Early in 1927 he had to choose a professor with whom to carry out the small research project required for his diploma (equivalent to a bachelor's degree). After much thought, he approached Professor Richard Becker, who accepted him for a project to check his new theory of metallic creep under stress. At first Boas was not too happy with the task assigned to him and his first tests were unsuccessful. Then, "Becker...came to the laboratory and gave me a proper dressing down in his wise and direct way which had a permanent effect on all my work: 'You must apply yourself with all your love and your whole soul to your project, otherwise no experiment will ever succeed'. How true this is and how often I thought of these words."

Boas praised Becker's personality, as one of the most ethical men he had ever met, with high principles from which he would not deviate and for which he stood up with great courage, even vis-à-vis the dangerous Nazis. When Becker (1887–1955) died in Göttingen, after a life marked by major contributions to nucleation theory and ferromagnetism as well as plasticity and even explosives, his memorial speeches all insisted on his striking honesty and uprightness of character. Heisenberg at the

Figure 14.4. Portrait of Walter Boas (courtesy of CSIRO, Melbourne).

time commented on the youthful rapport which developed between Becker and his students. It is also noteworthy that 6 years after his attention to Boas, Becker did the same for Egon Orowan, who also switched from electrical engineering to physics and studies of plasticity (see Section 3.2.3.2).

In later 1927, Becker saw to it that in spite of the severe Depression, Boas was given a job at the Kaiser-Wilhelm-Institut für Metallkunde in Berlin. Becker told Boas that he was dean of the faculty which had to adjudicate on the 'habilitation' (right to lecture at university) of a young Austrian metallurgist at the Institute, Erich Schmid, and that (in spite of his – Becker's – high ethical standards!) he would tell Schmid that he would agree to his habilitation only if he appointed Boas to a position in his section." He did, and was duly habilitated. On such curious practices can a lifetime career depend. With Schmid, Boas began the experiments on the plasticity of metal crystals (Sections 2.1.6, 4.2.1) that culminated in the publication, in 1935, of their joint book *Kristallplastizität*. Before that, in 1930, Boas obtained his doctorate (as Becker's first doctoral student); his thesis "created a small storm since it was the shortest ever submitted, 15 pages." Boas and Becker remained good friends, and in contact, for the rest of Becker's life.

Boas accompanied Schmid to the University of Fribourg in Switzerland in 1933, when Schmid was granted a chair there, and there they finished their book. Boas was lucky; he left Germany before Hitler took power. Though his parents were not observant Jews, and in fact Boas had been baptised, that would not have saved him from persecution. The Swiss, however, had a rule that prevented any refugee from staying beyond 5 years (which would give him automatic rights of permanent residence) and so Boas had to leave in late 1937. The committee in London that looked after refugees, run by the legendary Esther Simpson who has died only recently, found Boas a temporary haven with Sir William Bragg at the Royal Institution in London. Again with Esther Simpson's help, Boas managed to secure appointment to a 2-year Carnegie lectureship in metallurgy at the University of Melbourne in Australia, and in April 1938 he and his new wife left for Australia where he lived contentedly for the rest of his long life, becoming a citizen in 1944.

Boas's post at the University of Melbourne was made permanent, and for 9 years he taught and supervised research, and helped train metallurgists for war work. A number of noted metallurgists, such as Robert Honeycombe, passed through his hands. Then, after the War, the department was faced by insuperable difficulties and research facilities disappeared. In 1947 he applied for and secured a senior post in the Division of Tribophysics of the Commonwealth Scientific and Industrial Research Organization, CSIRO, also in Melbourne. 'Tribophysics' in the name was a residue of the interests of F.P. Bowden who studied wear and lubrication and sought a more elegant name to denote his interests (Bowden had moved on to Cambridge). Boas's duties were to undertake, and direct, research in the physics of solids. In spite of the tribophysics name, Boas took a broad view of his remit, and studied many aspects of metal physics. CSIRO made no difficulties about his choice of themes; they had an attitude to their senior scientists rather like that of Bell Laboratories... choose the best and give them their heads. How different from the situation today!

In 1949, Boas was appointed to the post of divisional chief after the incumbent retired. He took some persuasion to accept this, because it meant more attention to administration and supervision and would make it difficult for Boas to undertake personal research. But he accepted this and had an enormous influence on a whole generation of Australian physicists and metallurgists, aided in this by his open and affable personality. He remained in charge until 1969; his list of publications could not be large, though he brought out two more didactic books. He became known throughout the world; thus, in 1953 he became a senior adviser to the newly established *Acta Metallurgica*, and was invited to many international scientific occasions as a representative of his adopted country, which he defended fiercely against those who tried to slight it.

A book of scientific articles in celebration of Boas's 75th birthday (Borland et al. 1979) includes a biographical sketch of Boas by J.F. Nicholas. A substantial account of his life can be found in an obituary by Clarebrough and Head (1987).

After his retirement, the character of CSIRO changed utterly, and research in the Division, which repeatedly changed name, became wholly focused on applications. Boas's team fell apart and the scientific atmosphere in the Division became quite different. According to Clarebrough (2000), (one of Boas's most distinguished collaborators and the father of the first differential scanning calorimeter), "the decay of 'Walter's team' is a long story, but the main cause was a change in the politics of science funding in this country. CSIRO was hit first and now it has spread to the universities where funds must be raised for research from industrial sources and basic science is no longer funded." According to a news story in *Nature* (Swinbanks 1996) under the title "Basic research fighting for survival", the bureaucracy of science funding in New Zealand had by that year become 'horrendous' and applicants had to outline the expected outcome of their research. "This has encouraged them to pursue low-risk research rather than long-term fundamental research." Swinbanks went on to point out that Australia was headed in the same direction, but the story of Boas's Division suggests that it is already far down that path.

However, none of what has happened recently can detract from the contribution made by Walter Boas, that eminent physicist of solids, to the scientific life of his adopted and beloved country.

14.4.4 Jorge Sabato and materials science in Argentina

In 1955, being a Spanish-speaking metallurgist, I was invited to spend some weeks in Buenos Aires to deliver a course in elementary modern metallurgy to some members of the mainly youthful staff of the Atomic Energy Commission. The person who invited me, a dynamo of energy and originality, was Jorge Sabato (1924–1983) (Fig. 14.5), an Argentinian metallurgist who had recently joined the Commission's laboratory from local industry. I proved to be just the first of a procession of foreign experts, and later on Sabato organized more ambitious courses for which auditors came from all over South America. The Atomic Energy Commission came to be South America's leading focus of expertise in metallurgical engineering.

While I was in Argentina in 1955, Sabato took me to visit a brand new laboratory in Patagonia, deep in the 'south', near the ski resort of San Carlos de Bariloche. This was, and still is, the Centro Atomico de Bariloche (CAB). It is an institution (formally part of a local university) for research and teaching in physics, ranging from particle physics to solid-state physics. Its origin is one of the most curious in the entire history of academe.

Figure 14.5. Portrait of Jorge Sabato (courtesy of Heraldo Biloni).

In 1948, an Austrian physicist named Ronald Richter came to Argentina and managed to persuade President Perón that he knew the secret of cheap nuclear energy and, more specifically, cheap nuclear bombs. He was exceedingly tight-lipped about the details, but he sufficiently convinced the unscientific politician that he progressively accumulated money, laboratory space and extensive scientific equipment. Like the fisherman's wife of the fairy tale, he kept on coming back to the president's house, the Casa Rosada, to ask for more. In due course he was given exclusive use of an island, Huemul, on the lake of Nahuel Huapi, a beauty spot near Bariloche, a staff of engineers and masses of hardware; no visitors were admitted. Perón was taken for a comprehensive ride, and it was not till early 1951 that a brave 'real' physicist, José Balseiro, was able to persuade Perón to set up a commission of experts to inspect the island. They found that the project 'lacked scientific seriousness'. This phrase comes from a fascinating book that describes the entire history, both scientific and political, of this unserious episode (Mariscotti 1984, 1996).

After the commission reported, it took some time for the government to extract Richter from his island; surprisingly, he was allowed to retire peacefully and (I was informed at the time of my visit) to take up chicken farming near Buenos Aires. So by 1953, there was a mass of virtually unused laboratory equipment on the isle of

Huemul: what was to be done with it? Balseiro had plans for an advanced university institution, to be set up in comparative liberty far from the political quagmire of Buenos Aires, and persuaded Perón to make available a piece of land and some buildings on the shore of Lake Nahuel Huapi, just a mile or two from the island. This became the Centro Atómico de Bariloche, opened in 1954. Balseiro himself was a highly distinguished theoretical physicist. Sabato succeeded in persuading him to include metal physics in the syllabus of the Centro; he was able to convince the suspicious Balseiro that he did mean metal *physics*, not metals techology which would continue to be pursued at the Commission's laboratory in the capital city. A well-known Austrian physicist, Gunther Schöck, came to inaugurate this part of the subject-matter, the first of many foreign scientists who have enjoyed spending periods in Bariloche; that Schöck was an enthusiastic skier played its part in attracting him to this beauty spot. (There are some points of similarity between events in Melbourne and in Bariloche – foreign scientists played a crucial part in both places.) Sabato's diplomacy ensured that the CAB and the Buenos Aires laboratory thereafter worked closely together.

I came back in 1959 to deliver a course of crystallography lectures at the CAB, and by that time the metal physics was well established. It has continued to flourish, and broaden; many papers of note were published, and a succession of international materials symposia have been held there. The CAB director, Balseiro, died young, of cancer, and the latest of a succession of directors is José Abriata, an Argentinian materials scientist. Most observers, I believe, both in South America and beyond, would concur that the Bariloche centre is the most distinguished physics laboratory in South America. Materials science plays an important part there, and credit for that belongs to Jorge Sabato.

14.4.5 Georgii Kurdyumov and Russian materials science

The early path of scientists in Russia was not an easy one, especially for those precocious individuals who were far ahead of their contemporaries. In Chapter 3, I mentioned Federov, one of the three co-inventors of the theory of space groups in the late nineteenth century, who found no comprehension at home of his difficult ideas. Here I can also refer to Mikhail Vasilevich Lomonosov (1711–1765), an early Russian polymath, a scientist and littérateur, who took an interest in the whole of science as it was perceived in the Petersburg of his day. He insisted on the crucial bond between chemistry and physics long before Wilhelm Ostwald was born ("a chemist lacking knowledge of physics is like a blind man who seeks by touch"); he took an active part in improving glass technology in his native country; he put paid to the phlogiston theory well before Lavoisier did. These facts come from an as-yet unpublished essay on Lomonosov by a British science historian, Michael Hoare, very kindly made available to me. Hoare says: " We may without serious reservation identify (Lomonosov) as the first modern physical chemist, materials scientist, mineralogist, ceramist, research administrator and scientific educationalist, and still not nearly exhaust the rollcall of his activities." (In a more recent message, Hoare, 2000, expresses the view that some of the ideas credited to Lomonosov should really be laid at the door of Robert Boyle, a century earlier; their ideas are sometimes hard to disentangle.) Lomonosov had to spend too much of his energy in fighting political battles in the Petersburg Academy of Sciences; he was not the first nor the last to be so beset. But the man with whom I am mainly concerned in this Section did not spend his time in politics, and he had a huge influence on metallurgy and eventually on materials science in his country.

Georgii Vyacheslavovich Kurdyumov (1902–1996) (Fig. 14.6), the son of a priest, was the most famous metallurgist of his generation in the Soviet Union, a man who was not only a great research scientist but also a man of rare human qualities. He and the many people who collaborated closely with him spent decades on a single

Figure 14.6. Portrait of Georgii V. Kurdyumov.

broad cluster of problems; with some scientists, that would be evidence of a lack of imagination, but with Kurdyumov, it showed a deep and persistent curiosity and an ability to ask clear questions and to design crucial experiments that would answer them clearly. It is my great regret that I never had a chance to meet him.

Kurdyumov was educated as a physicist at Abram Ioffe's famous institute in Petersburg (= Petrograd = Leningrad = now, St. Petersburg). Alexander Roytburd, one of Kurdyumov's later collaborators, in a memoir of his revered master (Roytburd 1999), describes the Ioffe Institute as "the cradle of all soviet physics". (The 2000 Nobel Prize winner, Zhores Alferov, is currently director.) Roytburd goes on to claim that "working all his life in physical metallurgy, Kurdyumov kept close ties with the physics community and did a lot for the development of metallurgy in physical metallurgy, which is the fundament of modern materials science".

As a very young scientist, Kurdyumov homed in on the important problem of how and why carbon steel becomes hard when it is quenched from red heat. At an early stage, he established firmly that the hard phase was *martensite*, a distorted form of body-centred cubic iron with dissolved carbon. He studied the crystallography of martensite as a function of carbon content, took his diploma, and then in 1930 he was one of a group of 220 Soviet scientists who were allowed to spend a period abroad. He joined the German metallurgist Georg Sachs in Berlin; Sachs had found out how to grow single crystals of copper-based alloys, and Kurdyumov quickly found out how to convert this skill to the growth of crystals of alloyed austenite. Austenite is the (face-centred cubic) high-temperature phase – which by alloying can be stabilised at room temperature – from which martensite forms during quenching. He then cooled the austenite crystals enough for them to convert to martensite, and studied, by means of X-ray diffraction, the orientation relation between the two phases. This resulted in the celebrated Kurdyumov–Sachs relationship, still much quoted today. He also became convinced that the martensitic transformation (Kurdyumov's term) took place by a form of shear, without diffusion, and thereby initiated 70 years of intensive research on this type of transformation, in steels particularly (but not only in steels).

Back in the Soviet Union, he moved to the Ukraine to help, with his scientist wife, create a research institute in Dniepropetrovsk, where he continued with his researches. He was invited to be director, sought to escape from this fate (he complained that he would be a bad administrator, and that by administering he would lose contact with real science and then become unable to direct scientific work properly) but was persuaded to overcome his scruples. The rest of his long career he both administered (usually more than one institute at once) and remained a unique scientist. During the War, the institute had to move, and after the War, it was moved again, to Moscow, and Kurdyumov with it. While in Moscow, he also created a laboratory of metal physics in Kiev, Ukraine, and directed both the Moscow and the

Kiev institutes (Khandros 1992). In both laboratories, more and more subtleties of the martensite transformation, its crystallography, kinetics and mechanism, were undertaken, and Kurdyumov became internationally famous and established close links with American and Japanese scientists in particular. He and Khandros (Kurdyumov and Khandros 1948) published the first study in depth of a 'thermoelastic' phase transformation, the precursor of many later studies of shape-memory alloys (nowadays familar to many people in the form of 'shape-memory spectacles'), which are based on stress-induced martensitic transformations. I recall reading this paper in translation in 1948 and being astonished at its quality. The foregoing is only a rough outline of a few of the many profound studies that emerged from Kurdyumov's laboratories, resulting in almost 300 papers. Roytburd's (1999) panegyric goes into much greater detail. Kurdyumov remained director of the Moscow laboratory until 1978. His most important achievement was to train a whole generation of research metallurgists to a high standard, and to provide a model for them.

Two further aspects merit notice. Kurdyumov's Moscow laboratory was part of the great network of laboratories administered by the Soviet Academy of Sciences, and his Kiev one belonged to the Ukrainian Academy of Sciences. Throughout the Soviet sphere of influence, and also in China, the science academies were the chief organisers of scientific research – essentially, the academies were, and are, organs of state – whereas in the West, the academies are independent bodies of experts, ready to advise governments but not to administer laboratories. Briefly, just before the First World War, when the US National Academy of Sciences (NAS) was in its formative state, there were voices raised in favour of laboratories to be run by the NAS, but the idea was soon abandoned. Independence from the state was too precious to be thus compromised.

All who knew Kurdyumov well testify to his kindness, consideration of his staff and courage. Roytburd remarks: "In order to be a founder of a new scientific era one has to be a great scientist; to create a science school one has to be a great person. Kurdyumov was this scientist and this person. His personality attracted everyone who met him, but we, his pupils, colleagues and friends especially felt enchanted by him... He was Director of our institute but that was not what defined his authority. He was a spiritual leader because of his vision of the problem, his enthusiasm, his respect for the scientific truth, his belief that the truth is more important than success." Another of Kurdyumov's collaborators, Evgeny Glickman, informed me (Glickman 1999) that "my aunt who worked with Georgii Vyacheslavovich Kurdyumov in Dniepropetrovsk always stressed that at the peak of the Stalin terror, 1937–1938, Georgii Vyacheslavovich Kurdyumov saved her and many colleagues by answering for them at KGB with his own life. By no means was this safe – or typical – behavior at that time."

Throughout Kurdyumov's active career, metallurgy was taught in some places. semiconductors in others, ceramics in others still... there was no materials science. In 1985, encouraged by Gorbachev's perestroika and the opportunity for independent initiative which it brought, one courageous Russian professor, Yu.D. Tretyakov, who had earlier spent some time in Rustum Roy's laboratory at Pennsylvania State University (see the first paragraph of this chapter) and been fired by Roy's ideas, was able to set up Russia's first undergraduate course in materials science (nauk o materialakh) at Moscow's Lomonosov State University, in the form of a five-year programme. There is a degree of chemical emphasis, in view of Tretyakov's background, but on paper, as presented at a meeting at Penn State in 1999 (Tretyakov 1999, see also Tretyakov 2000), it seems a thoroughly well-conceived and balanced programme, and it appears to be attracting much competition for entry. This Section thus ends where it began, with awareness of the name of Mikhail Vasilevich Lomonosov. I would like to think that Professor Tretyakov was also in some measure fired by the personal example of Georgii Vyacheslavovich Kurdyumov.

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Chapter 15

Epilogue

Chapter 15
Epilogue

The time has come to draw together the threads of what has gone before. MSE is a huge domain; again and again I have had to warn the reader that I could only scratch the surface of some theme in the space available to me, and still I have covered more than 560 pages with a combination of history and depiction.

First, what is materials science? I have gone through my professional life almost without addressing this question explicitly; I have always believed that the right way to address it is by means of what philosophers call an 'ostensive definition', pointing to something and saying "This is it". This inclination was my main reason for accepting, in 1965, the hard labour of creating a new *Journal of Materials Science*; that journal was meant to demonstrate what my novel subject actually was, and I believe it helped to do that. This book is also an essay in ostensive definition. When I had just been appointed professor of materials science at Sussex University, I did write an article under the title 'What is materials science?' (Cahn 1965). Summarising my disquisition, I wrote: "...the materials scientist has to work at several levels of organisation, each of which is under-pinned by the next level. Here, again, he is brother under the skin of the biologist, who does just the same: starting with the cell wall, say, he goes on to study the morphology and economy of the cell as a whole, then the isolated organ (made up of cells), then the organism as a whole." I still hold today that this feature is central to our subject – applied to inanimate and artificial nature by us and to animate nature by biologists – and that the concept of *microstructure* is the most important single defining theme of MSE. To this can be added the slightly broader modern concept of *mesostructure*, a term particularly beloved of modellers and simulators of polymers... the level of organisation in between the atomic/molecular level and macroscopic appearance.

Merton Flemings, a very experienced professor of MSE at MIT, has recently discussed (Flemings 1999) the question: "What next for MSE departments?" He faces, foursquare, the issue whether something can be both a *multidiscipline*, bringing together for use many classical disciplines, and a discipline in its own right. He is sure that MSE is both of these. The path out of the dilemma "is to view the broad engineering study of structure/property/processing/performance relations of materials, with engineering emphasis... as a discipline". That is, he asserts, what mainline, independent MSE departments teach. This fourfold way is depicted in Figure 15.1(a), a little tetrahedron which was first proposed in a 1989 report. Flemings goes so far as to say that "our survival as a discipline and as independent academic departments within the university system depends on how well we succeed in articulating this paradigm and employing it to contribute to society". Others prefer to make this little diagram more complicated; thus Shi (1999), a veteran Chinese materials scientist, is insistent that 'composition' is an equally important variable, distinct from structure, 'processing' should be linked with 'synthesis', and at the heart of the whole enterprise he places 'theory and design of materials and processing', clearly including computer simulation. His view of things is shown in Figure 15.1(b).

One should not be perturbed by different experts' preferences for different kinds of polyhedra; after all, these are no more than a visual aid to understanding. The key thing is that different aspects are intimately related... in these figures, every point is linked to every other point. Each of these aspects, whether they be divided into four or six categories, needs a familiarity with some of the classical disciplines such as physics, chemistry, physical chemistry, and with subsidiary not-quite-independent sciences such as rheology and colloid science.

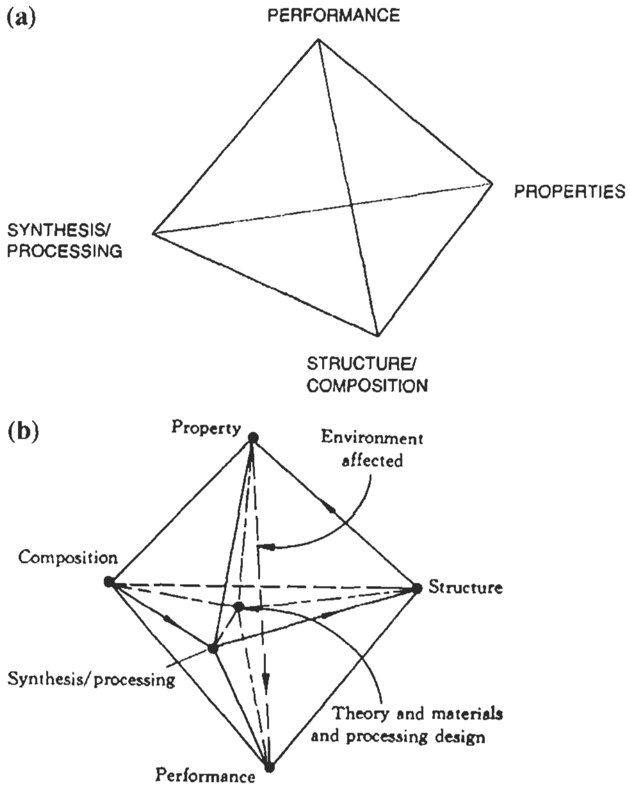

Figure 15.1. (a) The four elements of materials science and engineering, (after Flemings). (b) The six elements of materials science and engineering (after Shi).

While I entirely agree with both Flemings and Shi about the crucial importance of the components in their diagrams, I persist in my conviction that *microstructure* is the central component that best distinguishes MSE from other disciplines; each chapter of this book demonstrates this centrality. The other components in the diagrams themselves have microstructural features: thus self-assembled materials (a part of processing/synthesis) have carefully controlled microstructure, and composition, because of segregation, varies significantly from point to point – and all this intimately affects properties.

I recall my distinction, in Chapter 2, between emergence (of a discipline) by splitting and emergence by integration, and also my insistence that MSE is a prime example (together with geology) of emergence by integration. This is historically unusual. For instance, in a scholarly study of how chemistry and physics came to be distinct disciplines and then chemistry itself differentiated, Nye (1993) concludes (to simplify drastically) that around 1830 chemistry split decisively from experimental philosophy (or physique générale) by reference to its concern with molecules and their reactions and behaviour, and in doing so left physics behind. It is far harder to reach an acceptable definition of physics than of chemistry, but that has not prevented physicists from driving their discipline forward during the past two centuries. Likewise, we materials scientists practice our mystery whether or not we can define it.

So, nearly half a century after the emergence of the concept, we its practitioners have in materials science and engineering a clearly distinct discipline which in practice doubles up as a multidiscipline, with a substantial number of independent academic departments and research institutes spread around the world, with its own multifarious journals and textbooks, and a large number of professionals, also spread around the world, who call themselves materials scientists and engineers and communicate with each other on that basis. We have a profession to be proud of.

REFERENCES

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Flemings, M. C. (1999) *Annu. Rev. Mater. Sci.* **29**, 1.

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Shi, C. (1999) *Progress in Natural Science* (China) **9**, 2.

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Corrigenda

§ 3.1.2, page 72. Alois Joseph Franz Xaver von Beck-Widmanstätter, also known as Widmanstätten, was director of a 'cabinet' of manufactures for the Austrian emperor, not curator of a collection of meteorites. He was previously a printer, which no doubt gave him the impetus to use an etched section of a meteorite as a printing plate. He printed from other meteorites before he made the print from the Elbogen which is illustrated on page 73.

Recent researches on meteorites suggest that the cooling rates of meteorites with very coarse structures were typically some tens of degrees per million years. See C. Narayan and J.I. Goldstein, *Geochim. & Cosmochim. Acta* **49** (1985) 397.

In this same section (pp. 73–74) I discuss Henry Sorby's introduction of reflected-light microscopy of metals, later extended to rock sections examined by transmitted light; here I say that the Swiss geologist (Horace-Benedict) de Saussure ridiculed Sorby for venturing to "look at mountains through a microscope". De Saussure in fact died in 1799, 50 years before Sorby's first work with petrographic sections. What de Saussure did was to ridicule the 'pretensions' of 'natural philosophers' who discoursed on the origins of mountains without ever leaving their armchairs; it clearly seemed to him that looking at rocks through a microscope, if it were achieved, would amount to not leaving an armchair! The episode is discussed by D.W. Humphries in his chapter on Sorby, on page 17 of *The Sorby Centennial Symposium on the History of Metallurgy*, edited by C.S. Smith (Gordon and Breach, New York, 1965).

§ 3.2.1.2, page 110. Through an unfortunate oversight, I omitted to include here the reference I had intended to some very important early work on dislocation theory by the physicist Jacques Friedel (Paris); Friedel is mentioned in another connection on page 137. He was stimulated to work on dislocations by his stay in Bristol, 1949–1952. His contributions are recorded, together with others, in his book *Les Dislocations* (Gauthier-Villars, Paris, 1956), published in a thoroughly revised and updated English translation by Pergamon Press (Oxford), 1964. The personal background to his researches can be found in Friedel's autobiography (*Graines de Mandarin*, Editions Odile Jacob, Paris, 1994, pp. 169–179).

§ 4.2.1, page 160. In connection with Figure 4.3, of a spherical copper crystal following oxidation, it was mentioned that the sphere had been electrolytically polished. That technique (which can be simply described as the inverse of electrodeposition) has been vital for the production of strain-free metal surfaces for examination by microscopy; the most important pioneer in developing this technique was the French metallurgist P.A. Jacquet (see Jacquet, *Metallurgical Reviews* **1** (1956) 157).

Single-crystal turbine blades (mentioned at the bottom of page 165) are used not only in jet engines but also in some land-based steam turbines, notably those manufactured by GE.

An early overview of crystal growth can be found in a book by H.E. Buckley, *Crystal Growth* (Chapman and Hall, London, 1951).

§ 4.2.4, page 176. A useful adjunct to the history of crystallography is a *Historical Atlas of Crystallography*, edited by J. Lima-de-Faria (International Union of Crystallography, Dordrecht, 1990).

§ 6.2.2, page 217. Abbe, whose theory of diffraction-limited resolution is cited here, does *not* have an accent on his final letter. It appears that this is a common error.

§ 6.3.1, page 235. Clair Patterson's researches on lead contamination in the atmosphere, discussed in the last paragraph of this section, emerged from his earlier work on the age of the earth on the basis of precision measurements of concentrations of different lead isotopes, some radioactive, work for which he became famous. His definitive paper about this work is in *Geochim. & Cosmochim. Acta* **10** (1956) 230.

§ 7.3, page 281. Magnetic ferrites were first studied in Germany and then France, early in the 20th century, but no materials of commercially usable quality were found. This was first achieved in 1932 by a Japanese team, Drs. Takeshi Takei and Y. Kato, who developed a combination of magnetite and cobalt ferrite; the first patent was taken out in 1935, at the time when the Dutch work was just beginning. An account in English of this important early work in Japan can be found in a paper entitled "The Past, Present and Future of Ferrites", by M. Sugimoto, in *J. Amer. Ceram. Soc.* **82** (1999) 269.

§ 9.1.5, page 357. The seminar proceedings on ultrapure metals published in America in 1961 were preceded by a year by a French (CNRS) symposium on the same subject, centered on the researches of a chemical metallurgy group led by the influential metallurgist Georges Chaudron.

§ 9.4, page 367. Local minima in plots of grain-boundary energy versus misorientation, as seen in Figure 9.9 on page 371, are linked through the concept of DSC lattices (Displacement Shift Complete). A DSC lattice is defined as the coarsest lattice which includes the lattices of the two bounding grains (A and B) as sublattices; such a lattice is found for 'special' misorientations between the bounding grains. The 'less coarse' such an overarching lattice is, the lower the corresponding grain-boundary energy. The inverse of the proportion of lattice points common to A and B is called the sigma (Σ) number for that misorientation. This very influential concept was introduced by Walter Bollmann (*Crystal Defects and Crystal Interfaces*, Springer, Berlin, 1970), building on earlier ideas due to M.L. Kronberg and F.H. Wilson (*Trans. AIME* **185** (1949) 501).

§ 10.6.1, page 414. My statement at the bottom of page 416 that "the term 'icosahedral symmetry' is sometimes used" is inaccurate. That term is *always* used for the type of quasicrystals originally discovered by Shechtman, because these have not one, but six fivefold symmetry axes, like an icosahedron. Later, quasicrystals with only a single five-fold axis, combined with periodic stacking along that axis, were also found. Figure 10.7 does *not* show an icosahedral structure, but rather uniaxial tenfold symmetry.

§ 13.2.1, page 491. The 'Rubber Bible' (outlined on page 493) is now accessible online, with enhanced searching capabilities.

§ 14.3.1, page 512. A promising new broad-spectrum journal, *Nature Materials*, began publication in September 2002.

Epilogue, page 539. An important book by Mary Jo Nye concerning the emergence of disciplines is mentioned on page 541. Of several others which might have been added, I wish to cite a chapter by J. Dupré, "Metaphysical disorder and scientific disunity" in *The Disunity of Science. Boundaries, Contexts and Powers*, edited by P. Galison and D.J. Stump (Stanford University Press, Stanford, 1996) p. 101.

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