PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Computerized Materials-Information Systems [and Discussion]

H. Krockel, J. H. Westbrook, J. F. Barnes, R. W. Cahn, M. O. W. Richardson and N. Swindells

Phil. Trans. R. Soc. Lond. A 1987 **322**, 373-391
doi: 10.1098/rsta.1987.0058

Phil. Trans R. Soc. Lond. A **322**, **373–391** (1987)
Printed in Great Britain

Computerized materials-information systems

By H. Kröckel[1] and J. H. Westbrook[2]

[1] *Commission of the European Communities, Joint Research Centre, Petten, The Netherlands*
[2] *Sci-Tech Knowledge Systems, Scotia, New York* 12302, *U.S.A.*

Progress made in the development of computerized materials-information systems and current activities are reviewed both at the national level and internationally. Reasons for the lack of full realization of the opportunities offered by modern computers are elaborated and discussed. An intensified need for international collaboration and coordination is indicated.

Advanced materials, ceramics, plastics, intermetallic compounds, fibres, and composites, are appearing at an accelerating rate and there is strong demand for quick and reliable computer access to their properties. However, these new materials pose special problems for the data compiler and analyst: the properties and combinations of properties required are often new; there is a marked lack of standardization of materials, properties and test methods; the new materials are often not homogeneous, monolithic and 'off-the-shelf', but are rather *ad hoc* tailored compositions, micro- and macro-scale composite structures with strongly process-related properties; and there is increasing insistence by designers on property values of designated reliability.

The challenge is to accumulate data – numeric, tabular and graphic – from diverse sources, convert it to machine-readable form with a harmonized array of metadata descriptors and present the resulting database(s) to the user in a convenient and cost-effective manner.

1. Introduction

1.1. *Scientific and technical information*

It is noteworthy that the important intellectual activities of mankind – religion, art, philosophy, science – combine both creative and interactive elements, which, if dissociated, lead to ineffectiveness and sterility. Limiting the consideration to science, this dualism has accompanied the historical evolution from the Greek Academy of Plato, where the generation of medical, physical, philosophical and mathematical knowledge was intuitively combined with teaching as the most conservative and interactive form of knowledge dissemination, to modern research machinery, which combines highly sophisticated analysis methods with an equally sophisticated information technology.

This intellectual evolution is marked not only by the successive revolutionary effects of a number of technical inventions like the moveable-type press (the 'Gutenberg Revolution') and the computer, but also by major political, economical and sociological changes. Of particular influence have been the increasing specialization caused by the progressive division of labour and the intensified interaction of science and technology bringing about an unprecedented growth of applied research, the organized forms of which are nowadays largely conditioning the nations' technological and industrial capabilities and their economic efficiency.

As a result, scientific and technical information has itself developed into an important business sector and simultaneously has become a sensitive area of socio-economic concern (Toffler 1980; Schiller 1981; Naisbitt 1982; Williams 1982; AGORA 1983; Guile 1985).

Whereas the dissemination of fundamental research results has always been the classical domain of professional societies or scientific publishers whose business policies could be determined by the mechanisms of an existing information market, reporting the results of applied research has always been associated with market-adverse compulsions deriving from preconceptions of the possible use of results and the associated proprietary interests in control and exploitation by the user who has, at least, participated in defining the research program and often in funding the research at the source. Therefore, although one will accept that the flow of information generated by research follows the laws of an open market, there must be suspicion that applied research information has a market that is strongly distorted by special interests such as state control, subsidies, monopolies and various other restrictions. The economic aspects of the role of information in advanced technology are several: the information itself has a marketable value; it imparts added value to the product or process; and it accelerates the whole cycle from initial testing through development to final product. It is obvious that the influence of these factors does not diminish with evolution of the technical conditions for the storage and dissemination of information, the most far-reaching one being the progressive computerization of information services; on the contrary, their effects are markedly enhanced.

1.2. *The impact of computer and communication technology*

The traditional information service has been the library and its trained staff who assist the user. With the arrival of the computer has come the operation of brokered information services, for which the computer provides the attractive feature of enabling online access to electronically stored information as an advanced technical alternative to paper-based publishing, which is comparable to the alternative which the telephone offers with respect to written correspondence. In addition to computer storage, online operation also implies multi-users and remote access, features provided by telecommunication.

In the late 1950s the progress on systems providing online access began to support the expanding abstracting services which were established as a means to cope with the flood of primary literature. Bibliographic databases developed, and online bibliographic services made their public appearance; among the early ones relevant to the materials field are the National Technical Information Service NTIS (U.S.A. 1964) and Metals Abstracts Index METADEX (U.S.A./U.K. 1966). Today, the overall number of references related to materials, held by the world's bibliographic online databases is estimated to approach two million.

A more recent development of the late 1970s and early 1980s has been the personal computer (PC). In contrast to the online mode of access to computerized data, the personal computer offers the possibility of acquisition of customized files, creation of one's own 'electronic handbook', a sort of numerical samizdat, and a secure and inexpensive information resource.

Although originally limited in memory size and operational features, state-of-the-art PCs can now contain tens of megabytes of data, are enormously versatile and powerful manipulators of data, and can be placed on an engineer's desk for a few $1000. The most recent technological innovation, the compact disk CD-ROM (Pin-Shan Chen 1986; Oren & Kildall 1986) offers mind-boggling density of storage of information (the entire Encyclopaedia Brittanica on a single 5 inch disk), albeit with limited manipulation and search capabilities.

Whereas bibliographic databases are primarily designed for the provision of services and therefore have an *ab initio* association with online access, the second important category, called factual databases, can also have other purposes such as data management and processing, and may therefore be separated, both conceptually and actually, from the online concept, although online access is still a possible mode of use. The term 'factual' means that such bases allow retrieval of facts, i.e. information in the form of specified numbers, words and composite numerical and verbal assemblies. In Eastern literature, the distinction from the bibliographic base is made by the expression 'factographic', a term that is pertinent and merits adoption.

Factual online services have operated thus far in the public market mainly in fields like finance, business, economy and trade. Factual data of scientific and technical nature have been extensively processed and stored in computer databases for private use but have infrequently been offered online. Previously, memory size and data structure complexity requirements of databases and of application programs of technical interest so far exceeded capacities of the early PCs as to make them impractical, today's machines are creating a new market for offline, machine-readable information. Typically a vendor combines both data and selected application programs on one or a pair of 'floppy disks' that may well service most of an individual user's daily needs. Such products are now offered by both professional societies such as American Society of Metals (ASM) or commercial enterprises such as Engineering Science Data Unit (ESDU) and together with the CD-ROM constitute an entirely new, and perhaps ultimately dominant, technical information market.

Science and technology may have ultimate benefit from the development of a third category of information source, the knowledge base, which uses identical hardware but incorporates special software programs from the domain of so-called artificial intelligence. Such knowledge-based systems open the possibility for computer-assisted intelligent evaluation, advice, reasoning and decision-making. Because such capabilities will also be required by the user interfaces of factual bases, and vice versa because knowledge bases also need data, the future is likely to bring us various combinations of these concepts (Dixon & Simmons 1983; Hayes-Roth *et al.* 1983; Weiss & Aha 1984; Sargent 1985; Sowizral 1985; Swindells & Swindells 1985).

The use of databases for online services requires remote access that is provided through communication networks. The main development enabling high-volume digital data flows to be processed economically over long distances is the packet-switching technology that is used today in all networks based on private as well as public circuits. In the United States, private networks such as Tymnet and Telenet have been the main development; in the European Community, where PTTs (poste, télégraphie, téléphonie) hold monopoly positions, the introduction of public networks has been underway since 1975 with the development of the EURONET–DIANE system. EURONET has in the meantime been replaced, as planned, by the international linkage of the European national packet-switched networks. The U.K. packet-switched service (UKPSS), for example, was introduced in 1981. DIANE (the direct information access network for Europe) links host computers in the European Community where more than 800 databases are operating.

2. Materials Data Systems

2.1. *Background and development problems*

Among the categories of applied research information that have a pronounced sensitivity to socio-economic factors are the properties of technically relevant materials. Factual data on materials and their properties are the most condensed form of materials information needed in engineering technology, and it is not surprising that they are considered as vital resources for the competitiveness and innovational capacity of industry. This critical potential of materials information has actually been widely perceived and has given rise to world-wide efforts driving the enhancement of generation, evaluation and dissemination of materials data and knowledge (Westbrook & Rumble 1982; Brown 1983; Kröckel *et al.* 1985; Ambler 1985; Westbrook *et al.* 1986; Reynard 1986).

As part of these efforts, increasing emphasis is allocated to the rationalization of the information processing and transfer capacity of factual materials information systems. Materials-related factual data systems that are approaching maturity have not necessarily been designed for operation on the open information market but have more usually been intended for usage between and within organizations and even as components of integrated information and analysis systems linked with a laboratory or an analysis centre. The background of these systems can therefore be separated from the driving forces of the information market, all the more so considering that the main problems of their developments are in the peculiar nature of the materials information itself (Dathe 1985; Westbrook 1985*a*).

Factual databases also differ in character from bibliographic databases in a way that affects both their marketability and the technology used to store and access the information. Factual databases are 'living', constantly being updated, and refined in contrast to bibliographic databases, which are archives, 'frozen in time', and not subject to improvement or change.

Depending on the degree of sophistication one wishes to use in the analysis, a single property of an engineering alloy determined by a typical material test can be shown to be influenced by several dozen parameters that have their origin in the characteristics of the material and its production processes, the test method and conditions, the testing controls and environmental parameters, the specimen characteristics, and in various technical, commercial and standard conditions. Collectively, these descriptors of the numeric property data themselves are known as 'metadata', data about data (McCarthy 1982; Shoshani *et al.* 1985). The ways in which the physical and technical parameters influence each other and the property under consideration are complex and sometimes even poorly known, in addition to the problem of their quantity. Unlike the fundamental scientist who tends to simplify and isolate effects to study causalities, the engineer lives with a pragmatically optimized multiparameter system. His materials are not only subject to physically accessible factors, but also to those relating to production technology, trade, legislation, safety and standardization (Bullock *et al.* 1986). The way in which these complexities affect the flows of data and knowledge to the ultimate engineering user is shown schematically in figure 1, which also differentiates between raw, validated, catalogue, standard and evaluated data.

An adequate formal description of a computerized materials data system, or of a relevant, self-consistent subsystem satisfying the information requirements of a limited technical application, therefore requires much analytical effort. The resulting complexity has usually made the computer implementation of engineering material data systems very demanding, and finally expensive, enterprises.

An example of an analysed structure of information groups and influence parameters (metadata) for a typical scope of material properties that are presented as test results is shown in table 1, which depicts the data structure of the High-Temperature Materials Data Bank of the CEC Joint Research centre (CEC 1983; Fattori *et al.* 1985). The structure is characterized by five classes of data that are treated as logical units.

This logical structure can be translated into computer representation in the form of 'files'

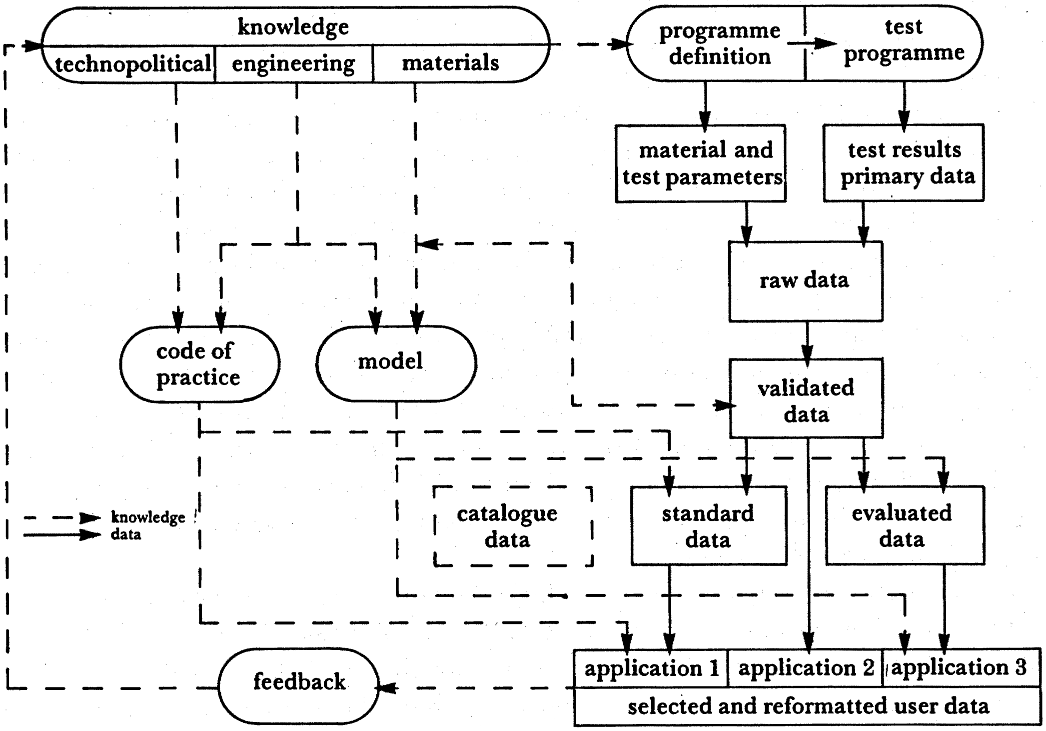

FIGURE 1. Data and knowledge flow chart for engineering materials properties.

TABLE 1. DATA FILE STRUCTURE OF THE HIGH-TEMPERATURE MATERIALS DATA BANK OF THE CEC JOINT RESEARCH CENTRE

test result

- tensile
- creep
- hot work
- relaxation
- fatigue
- creep crack growth
- fatigue crack growth
- toughness
- corrosion
- erosion

material	specimen	test condition	data source
designation	identification	temperature	corporate source
production	geometry	environment	author(s)
composition	production	loading	publication title
thermo-mechanical treatment	thermo-mechanical treatment	pre-test exposure	book, journal
hardness	hardness	test method	publisher
grain size	grain size	standard	date
microstructure	post-test analysis	test equipment	patent
RT properties	fracture mode	laboratory	project
physical properties			

that can be considered as the analogue of a set of data sheets structured according to the same logic. In practice the equivalence of these two logics is necessary to achieve the input of data by means of so-called data collection forms. The achievement of organized data storage, which must enable (and preferably facilitate) retrieval, requires a structured coding system that corresponds to the application of a numbering and linkage principle to all elements of the data bank. Such a scheme not only connects the paper records directly to the computer files but also serves as the basis for an 'audit trail' should the source or history of any individual property value be questioned.

The possibilities of data retrieval depend on the quality of the structural design, the structured coding system and the database management system. The level of sophistication of these components, however, also affects the cost of data banks, a factor that must ultimately determine their creation or continued existence. It must be clearly realized that high costs are not only involved in their construction but also in their operation, in particular in the input and output interfacial processes. The problems and costs caused by the formatting and input of data often prevent the commercial feasibility of a computerized database. Equally there are many unsolved problems at the data output end of the system where communication with materials specialists or engineering users takes place (Fattori & Krefeld 1987). The development of intelligent access procedures and query languages, which relieves untrained users of the need to acquire detailed system knowledge, is far from a satisfactory status. The resulting poor usage, in combination with the high cost of the data input process, causes, for many systems, a prohibitively bad cost-effectiveness.

Analyses of other underlying reasons for little use of existing materials databases, aided by several industry-focused workshops (Rumble & Westbrook 1985; Rumble & Northrup 1986; Rumble 1986; Kaufman 1986; Westbrook & McCreight 1986), has revealed several generic user needs that must be largely satisfied before computerized materials information systems can become an effective engineering tool. These needs may be summarized as follows.

Comprehensiveness. The system must include not just many properties for a few materials or a few properties for many materials but a scope of such breadth in both respects that most of the average engineer's needs are met. Thus a pragmatic but not an absolute comprehensiveness is demanded.

Reliability of data. Data of the highest reliability are always sought, but, in any event, the character or reliability of each number shown must be presented, for example, minimum, maximum, typical, standard, 95/90.

Full complement of metadata. All relevant material, property, test, specimen and other descriptors must be included from laboratory records or print sources. Typically this means 10–100 ancillary items (quantitative and qualitative) for each property value.

Ease of system use. The information system should be no more difficult for engineers to use than their telephones. In particular he must not be forced to learn the idiosyncracies of several different systems or subsystems in order that all his information needs be served.

Versatile, integrated capabilities. The system the engineer wants should combine number and fact look-up with calculational and manipulation capabilities, ex-system referral, customized graphic and tabular display options and possibly full text retrieval of cited documents, for example, standards.

2.2. *Progress towards operational systems of engineering use*

The mentioned drive to enhance the generation, evaluation and dissemination of materials information has given rise to various efforts to overcome the inherent problems of materials data information previously reviewed and create feasible systems of general engineering use (see, for example, Graham *et al.* 1980; Westbrook 1982, 1983). These efforts are essentially incited by two technological trends:

the removal of technical barriers by progress in information technology, telematics, software, low-cost equipment and standards;

the growing demand for computerized materials data caused by the computerization of engineering methods for design, analysis and manufacturing (NBS 1984).

It is recognized that the economically disastrous lack of use of the few existing data banks is caused by the technical problems of their development as well as by external factors such as an underdeveloped behavioural inclination to the use of computers and the requirements of comprehensiveness cited above. Comprehensiveness can only be generated in practice by integrating databases of limited scope into large systems. The need for maintenance of specific data scopes by expert teams suggests, not that a superdatabase be created, but that effective comprehensiveness be generated by networking distributed databases. Consequently, the concept of materials information networks is finding interest, and it also appears to provide solutions for certain other problems of the field.

Networks combining incoherently developed databases of autonomous institutions require cooperation in developing suitable structures for coordination and management, in particular in international environments. A number of international meetings and workshops has prepared the ground and created a positive atmosphere for cooperation:

the Fairfield Glade Workshop on computerized materials data systems in 1982 (Westbrook & Rumble 1982);

the Petten CEC Workshop on factual materials data banks, in 1984 (Kröckel *et al.* 1985).

The Schluchsee CODATA Workshop on materials data systems for engineering, in 1985 (Westbrook *et al.* 1986).

The most severe handicap for the development of factual materials data systems and information networks for an international scope of operation is the inadequate level of agreed, harmonized standards for materials, tests and properties. It is obvious that the intermediary function that data storage in a computerized database has between an environment that generates data and an environment that uses them makes the use of unambiguous terms and descriptors necessary. The call for a world-wide multilingual standard terminology for the materials field including definitions, symbols and abbreviations is therefore brought forward by materials data banks stronger than ever, as is the general need for clear standards in materials designations and numbering systems as well as test methods that define the properties to be processed.

As one consequence, a working group of the Versailles Project on Advanced Materials and Standards (VAMAS) has been charged to foster communications between these activities and to assess the sufficiency of all the international standards needed to build materials data systems. A further result is that the American Society for Testing and Materials (ASTM) in March 1986 organized a new main technical committee, E49, to address standards and terminological issues related to the 'computerization of materials properties data'. The accentuated need for standardization of terminology caused by computerization was also emphasized by Westbrook (1985*b*) in a study of several groups of mechanical property tests in which consideration was given to definitions, synonym lists, data reporting standards, and standard reference materials among other issues.

2.3. *Database networks*

Athough these world-wide approaches to large-size national and international materials data networks are conceptually designed to match the users' need for interactive, remote access to comprehensive information, their initial realization depends on the incorporation of currently available databases which have already reached an operational status. Practically all these existing databases have been developed without coordination and therefore represent a very heterogeneous system of data scopes, structures and other features. The European potential of materials database projects including only publicly available information is estimated to be of the order of 50, of which 10–20% may be mature enough for online operation in a materials data network. The initial group of candidate projects for a European-Community organized 'Demonstrator Programme' establishing a pilot network consists of 11 databases covering mechanical, physical, thermodynamic, corrosion and other engineering properties of ferrous and non-ferrous alloys, plastics, ceramics, composites and powder-base materials (Kröckel & Steven 1986, 1987).

In the United States similar activities are underway: two networking experiments – the Materials Information for Science and Technology (MIST) system sponsored by NBS and the Department of Energy, and the National Materials Properties Data Network (NMPDN) initiated by the Materials Properties Council; and privately offered groupings of chemically related databases such as those by Technical Data Services, Inc. (TDS) and by Chemical Information Systems, Inc. (CIS).

For the MIST project, properties of about 175 widely used alloys were selected for incorporation into a prototype network system from three frequently used, printed sources of high reliability, already in the public domain: *Aerospace structural materials handbook* (ASMH), *Structural alloys handbook* (SAH) and *DoD Military handbook V. A project overview* (Grattidge *et al.* 1986) has been prepared which anticipates a phased approach to a network system of progressively increasing heterogeneity as summarized in table 2 and described more fully in a recent report (Northrup *et al.* 1987).

TABLE 2. SCHEMATIC SCHEDULE FOR BUILDING A VERSATILE, DISTRIBUTED MATERIALS DATA NETWORK SYSTEM

phase	data sources	data structures	computers sites	hardware operating systems	DBMS (database management system)	user interface
I	one	one	one	one	one	command
II	multi	one	one	one	one	elem menu
III	multi	multi	one	one	one	combined
IIIa	multi	multi	pass through	one	one	simple gateway
IV	multi	multi	multi	one	one	PC-based
V	multi	multi	multi	multi	one	full gateway
VI	multi	multi	multi	multi	multi	expert system augmentation

Kaufman (1986*a*, *b*) has described NMPDN as a not-for-profit corporation organized to provide 'ready online computer access to a wide variety of reliable research and engineering data on the properties of materials'. The corporation is supported by a broad range of industrial companies and some government agencies. It is planned initially to link existing machine-readable U.S. materials databases, then add other machine-readable databases that could be incorporated with minimum effort and finally to seek means for creating entirely new databases that would fill holes in the then existing network. Initial emphasis will be on design mechanical properties with their supporting metadata.

2.4. *Some new features*

Modern computerized information systems have, or will soon have, additional features that will make them more attractive and useful to the practicing engineer. The first that we shall mention is the presentation of graphics. From simple presentation of linear x–y plots we have now progressed to: automated conversion of units and scale type; incorporation of 'zoom' capabilities; and three-dimensional plots with the possibility of horizontal or vertical sections through them. Another feature is a referral directory, available on call, to supplement the data stored in the system itself with referral to a supplementary print data source or an individual expert on the subject property or material. Ultimately this trend may lead, in the case of a multiterminal work-station to a means, perhaps via CD-ROM, of immediate access to a full text reference source, for example, a referenced specification or a materials encyclopaedia. Finally, there is the possibility of recovery of so-called derived properties, calculated on demand from stored algorithms. Examples are specific strength (strength divided by density) or thermal diffusivity (thermal conductivity divided by (specific heat multiplied by density)).

3. INFORMATION AND ADVANCED MATERIALS

3.1. *Background*

Before World War II, materials developments occurred in the familiar patterns of increasing diversity of useful materials within traditional classes, improved properties of familiar materials, and enhanced control and efficiency of materials processing. In attempting to meet the challenge of new fields of application (space, electronics technology, atomic energy) and to exploit new scientific understanding, materials development has left the evolutionary stage and entered a revolutionary era.

Although we may speak of ceramics, plastics, intermetallic compounds, fibre reinforcements, superalloys and composites as representatives of classes or subclasses of advanced materials, these names do not reveal the striking differences in form, structure, properties and processing of new materials from those of the similarly titled classes of traditional materials. Furthermore, from a classification viewpoint how are we to regard an advanced material (AM) consisting of an aligned array of TaC fibres in a multicomponent superalloy matrix prepared by directional solidification of an eutectic, or an integrated electronic circuit containing thousands of resistors, conductors, insulators, transistors, etc. produced *in situ* by multistep physico-chemical processing rather than by assembly from discrete components?

It is at once apparent, even from this brief introduction, that two factors have, in concert, prevented the incorporation of numeric data on advanced materials into traditional printed handbooks:

the rapidity of the development of AMS;

the inextricable integration of processing and materials composition in fixing properties of AMS, i.e. many, if not most, AMS are not so much materials as multimaterials systems whose properties depend strongly on internal interfaces and external joints.

Whereas those same factors are operative with respect to incorporation of any materials data in the new computerized numeric databases, the rapid updating capability of computerized systems and their ability to cope with a very large number of independent variables affecting properties should encourage this approach to the creation of information sources on the properties of advanced materials. Problems abound, however, as evidenced by the present lack of computer access to properties of these materials. Many examples are included in published lists (Hampel *et al.* 1984; Schwartz *et al.* 1985; Westbrook *et al.* 1986), but it is notable that few databases focused on AMS are publicly available. Although data collections on AMS intrinsically contain information of a proprietary nature, even in-house systems require organized machine-readable databases. It must also be recognized that much relevant data on AMS are not themselves proprietary and if standardized and harmonized, could be made available to public databases or networks without jeopardy of commercial interests. The next sections will review some of the problems in building databases on AMS.

3.2. *Standardization*

The urgent need for standardization in several aspects of any computerized materials systems has already been discussed. This need is even more acute for the advanced materials (AMS) because, as compared with traditional alloys and ceramics they are not well standardized in any respect. There are several aspects of this lack of standardization that influence the characterization and designation of AMS:

AMS are not compositionally defined;

with AMS, the product often determines the properties and the properties define the material rather than the traditional inverse order;

AM properties are process dependent;

defects in AMS are definitive;

AMS are usually anisotropic;

AMS are inhomogeneous materials.

On both a micro- and a macroscale, AMS are often composite materials and must be so regarded. Reported properties therefore usually relate to exceptionally homogeneous test specimens and not to actual products of the same nominal material whose composite character may vary across a cross section or from point to point in the part as a circumstantial result of processing or from a deliberate intent to locally tailor properties.

The challenge then, for the AM producers, users, and information system builders is to introduce some agreed-upon standardization for these materials, their designations, production processes and properties, which will be definitive and unambiguous, analogous to the Unified Numbering System (UNS) of ASTM/SAE for metallic alloys, even if not compositionally based.

Standardization of test methods, both nationally and internationally, is always highly desirable, and nowhere is this more needed than in AMS such as plastics and ceramics. An illustration of the acuteness of the problem may be found in a recent paper by Quinn & Boratta (1985) who report over 100 'standard' test methods for determining the flexure strength of ceramics. The major test variables found in their survey included: loading type (three point against four point), loading rate, test span, specimen size and aspect ratio, and specimen preparation. Errors, or variability from test to test for the same material, in the range 20–100% of the measured value, are common. Although there are difficulties in applying traditional test methods to the AMS as just illustrated, the problem of standardized test methods becomes even more acute with reference to newly required property measurements, a subject to which we next turn.

3.3. *New properties and independent variables*

In attempting to apply AMS in new and more demanding environments, engineers have found need for access to quantitative values for new parameters such as those that characterize a

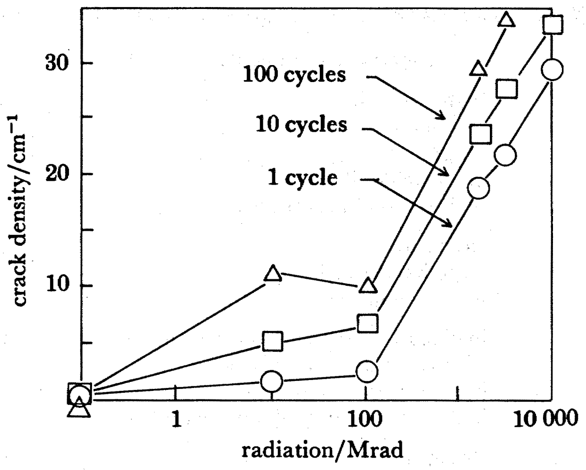

FIGURE 2. Resistance to microcrack formation of graphite–epoxy laminates subject to long-term irradiation exposure and thermal cycling in space (Klein 1986*a*).

material's resistance to thermal shock, to slow crack propagation or to irradiation. An example shown in figure 2 illustrates the type of materials data needed to build a space station, for example, the resistance to microcrack formation of graphite–epoxy laminates subject to long-term irradiation exposure and thermal cycling in space (Klein 1986*a*).

The large number of independent variables affecting common properties of AMS has already been alluded to. The difficulty can be illustrated more explicitly by considering the mechanical properties of a typical fibre-reinforced composite. The fatigue strength of such a material, even for a fixed reinforcement-matrix combination at a fixed reinforcement size and volume fraction, has been found to vary markedly with the nature of the coupling agent used, the fibre orientation, the style of weave and the mode of introduction of the fibre (prepreg against woven against filament wound) (Klein 1986*b*). An analogous example showing the effect of orientation with successive plies of layup of a laminate on the fracture toughness (mode 1, initial strain energy release rate (G_{Ic}) is shown in table 3.

TABLE 3. EFFECT OF FIBRE ORIENTATION IN A MULTI-PLY GRAPHITE–EPOXY COMPOSITE ON FRACTURE TOUGHNESS (PEEL TEST) (KLEIN 1985)

material	ply layup orientation in degrees (number of plies)	$G_{Ic}/(\mathrm{J\ m^{-2}})$
epoxy	0(24)	471
epoxy	+45/−45/0(8)/−45/+45/ −45/+45/0(8)/+45/−45/	600
epoxy	+45(2)/−45(4)/+45(2)/ −45(2)/+45(4)/−45(2)/	1400

These examples illustrate how complete and exacting the material and test value descriptions must be if comparisons are to be valid and design calculations meaningful.

Certain properties required for AMS are new in the sense that they reflect the probabilistic nature of failure in these materials. Examples include the so-called Weibull analysis of fracture

Table 4. New combinations of required material properties

application	property requirements	material
submarine hull	high strength low density toughness good weldability high corrosion resistance	titanium alloy
fibre optics for communications	strength large band width low attenuation	silica glass
nuclear-reactor fuel cladding	low neutron absorption cross section high thermal conductivity high corrosion resistance high strength at moderate temperatures	zirconium alloy
artificial heart valve	strength impermeable biologically compatible immune to biological degradation	pyrolitic carbon

in ceramics and other brittle materials or the measurements of crack growth rate as a function of stress state and environment necessary for many high strength materials in critical applications.

Other properties are new only in the sense that a new field of application for materials has required a combination of properties not previously sought, as illustrated in table 4. However, if comparison is to be made of candidates, even more conventional materials, all pertinent properties must be available or determined *ad hoc*.

4. Drivers and trends

4.1. *The demand for computerized material databases*

There are a number of current advances in both materials science and engineering on the one hand and in information technology on the other which are acting as drivers for the creation of computerized databases for materials. At a minimum such a resource would considerably facilitate any new engineering technique or assist in the application of a new material. Sometimes, however, the new technique absolutely demands the availability of a computerized database if it is to be effective. The subsequent sections review briefly the more important of these drivers and trends.

4.2. *Accelerating tempo of materials development and application*

Whether we look at structural materials, bio-materials or electrical materials, it is clear that the tempo of transfer of materials technology from the laboratory to application is increasing rapidly. Improved information is both cause and effect of this phenomenon. More data must be captured, evaluated, stored and made accessible more quickly than ever before. The impracticality of a long experiential, cut and try stage in modern engineering systems in turn demands large databases for computer modelling and better means of predicting material performance. Reciprocally, the more success achieved in these respects, the faster the transfer of materials technology to application leading to a new demand for better and more complete materials information.

4.3. *Criticality of materials performance and reliability*

Many engineering systems today impose extreme new levels of reliability for materials and hence on the reliability of properties information on them. These requirements stem from three sources: the very large dollar value of certain engineering systems, for example, the space shuttle at over $\$10^9$ per copy; the inaccessibility for maintenance or repair, for example, nuclear reactor core or artificial human heart; or ultra-long term performance measured in decades or centuries, for example, power stations or nuclear-waste entombments.

4.4. *Computer modelling*

The use of a computer, given the proper algorithms and data input, to simulate the behaviour of a device, system or material is known as modelling. A particular instance in the engineering field is the finite element technique that has been applied to stress analysis, heat transfer and electromagnetic field analysis. For any of these programmes to yield useful results, a rich database of materials properties must be available including not simply the property values at nominal or default conditions but as a function of temperature, frequency, anisotropy or other relevant variables. Here again a computerized database is virtually required to make these analyses practical and meaningful. Computer modelling also applies to materials data themselves, independent of the particular engineering application, component or system. In this case the attempt is made, by using the computer's powerful calculation and display capabilities, to express the behaviour of, for example, a large set of stress–strain data, or several such sets, by some empirical or theoretical parametric formulation, a so-called 'constitutive law'. Establishment of such conformance can:

effect considerable compression of data from diverse combinations of independent test variables to a simple, concise representation of the behaviour of a given material;

provide an analytical formulation of the material behaviour for input to stress analysis, for example, by finite element methods;

enable life prediction of components or systems;

help verify theories of the behaviour of matter;

permit interpolation, and sometimes extrapolation, from the experimental data to include conditions not physically tested;

help identify regularities and patterns in data leading to new models and new theories;

help guide experimental research in fruitful directions, often reducing the number of test measurements required;

facilitate the simplification of an experimental program and hence effect economics in development, by making possible computer simulation of materials behaviour.

This more advanced stage of a computerized data file is sometimes referred to as dynamic data bank use, as contrasted to the more conventional static data bank developed in the early stages. A dynamic use concept of the data bank is shown in figure 3, which is an amplification of a particular part of the general schema of knowledge flow in figure 1.

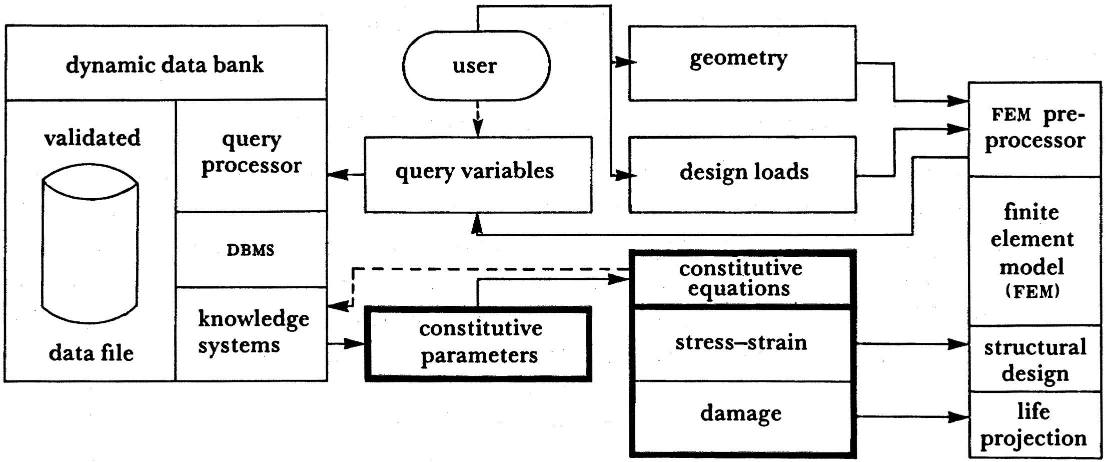

FIGURE 3. Conceptual scheme for the linking of a materials properties data bank with stress–strain–life analysis by finite-elements computation.

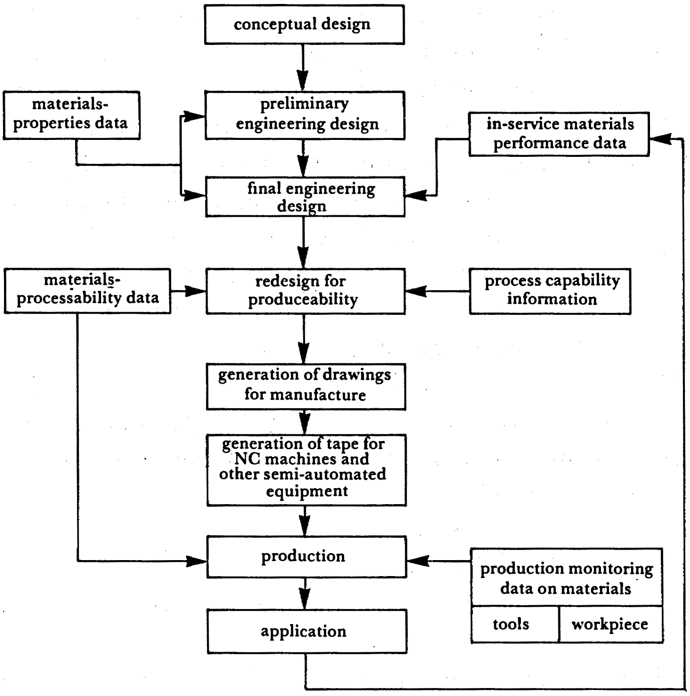

FIGURE 4. Conventional engineering–manufacturing flow chart.

4.5. *The engineering workstation*

A generation ago the engineering–manufacturing flow chart was approximately that illustrated in figure 4 with various types of materials data required at different points in the cycle as indicated. These numbers could be provided as needed from various handbooks or private files: the usual time scale and the segmented nature of the process permitted this casual and uncoordinated data input.

Today computer-aided design (CAD) (once only an automated drafting operation) is being extended to a fully integrated function, computer-aided engineering (CAE), which in turn is merged with computer-aided manufacturing (CAM) now maturing to computer-integrated

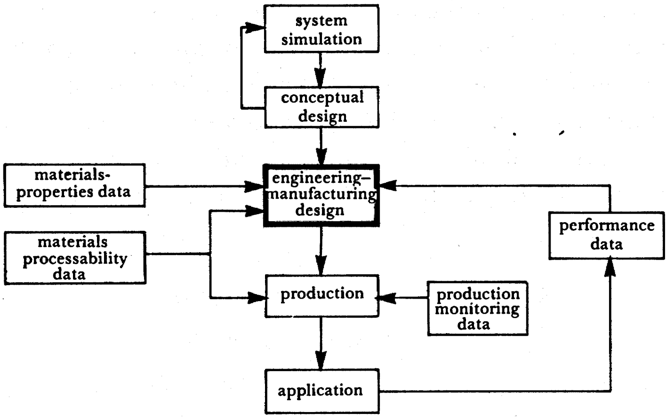

FIGURE 5. Integrated engineering–manufacturing flow chart (engineering workstation concept).

manufacturing (CIM) to constitute an almost totally automated and integrated process. (Salzman 1985). This compression and integration of the engineering–manufacturing cycle, aided by the possibility of preliminary computer simulation of component or system performance, is shown schematically in figure 5.

With this schema, the core information device with its associated databases is known as the engineering workstation (Joy & Gage 1985). From such a station an engineer can design a part, select a material, plot component performance, estimate life, generate machine-readable instructions for production equipment, etc., all in a continuous, interactive mode. For the full potential of the workstation to be realized requires a materials database that is more complete, more precise, more fully harmonized and instantly available than anything that has come before.

4.6. *Integrated computerized design*

The most advanced and complex engineering systems of today require an entirely new approach compared with the traditional one. Whereas previously in designing an airplane, for example, the aerodynamic design, the structural design, that of the propulsion system and the materials requirements for each, were considered more or less independently, today, in the U.S. National Aerospace Plane R&D programme (Heppenheimer 1985) to develop an ultrahigh-speed plane involving supersonic combustion ram-jet propulsion, liquid hydrogen fuel and cooling, and computer-governed controls, the design aspects of materials, form and function are inextricably linked and must be solved simultaneously by using supercomputers. It is obvious that new demands are placed on the materials database to support such an approach.

4.7. *Expert or knowledge-based systems*

Expert or knowledge-based systems, already alluded to in §1.2, are intended to use the computer, with associated software and databases, to emulate human reasoning to solve complex technical problems. Such systems incorporate several distinct elements: first a large store of facts, both quantitative data and qualitative descriptions, statements and observations. Here it is important to include record of negative experiences – what did not work and why, as far as it is known – as well as positive statements and data. Second, a number (often very large) of rules of inference pertinent to the scope of application of the program, for example, 'if this is so and that is so, then x is the result'. Finally, a number of interactive features between the user and the computer system that are invoked: at the outset of the session to help formulate and sharpen the query, throughout the process as various subprograms or loops are exercised, and at the end when the user wishes to review the logic trail by which the computer program reached its conclusion. Such systems are expected eventually to have particular application to and impact upon advanced materials developments because of the very large number of possible materials choices, the large number of variables affecting material properties and the complexities of the environments in which advanced materials are to operate.

5. RECOMMENDATIONS AND FORECAST

5.1. *Standardization needs*

There is no one factor more important to enhancing the capabilities and use of computerized materials information systems than a marked increase in the degree of standardization, both in the sense of uniformity and harmonization and in the sense of a minimal level of acceptability of data. This is particularly needed for advanced materials. As detailed in the body of the paper we need standardization of materials, of terminology, of data test records, computer file structures and of data presentation modes in the literature.

5.2. *Demonstration programs*

Over the past ten years, many experiments and much writing on the subject of computerized materials information systems have failed to produce a system that is widely used or even one that is demanded by a significant body of engineers. The fault lies not with the technology but with inadequate funding and coordination. Ten duplicative, fragmentary and uncoordinated $200000 projects are in no way equivalent to a single, comprehensive, integrated coordinated effort at a $2 million level. The demonstration programmes now at their inception, the NMPDN in the United States and the EC's Demonstrator Programme in Europe, bid fair to lead us out of this vicious circle, by demonstrating to engineers and management alike that the power of a comprehensive, well-planned materials information system would easily justify a several million dollar effort.

5.3. *'Dynamic' materials information systems*

One factor that may constitute the catalyst for a breakthrough is the evolution from static to dynamic systems that begin to incorporate features of so-called expert or knowledge-based systems and to provide an increasing number of user-interactive features. Such changes would vastly improve the power, attractiveness and ease of use of the systems.

5.4. *Customized information systems*

The advent of the personal computer has opened the way for a truly customized materials information system, both in respect to the data it contains and the array of available application programs. Again standardization in all the respects cited above would help make customized systems a reality. If this forecast is correct, the online systems confidently expected a few years ago may only come to be one of several access modes for the individual user of numeric data. In particular, online operation may provide the interlinkage of autonomous databases from which an information intermediary (professional society, trade association, nation or individual entrepreneur) will create the customized packages the market will demand.

5.5. *International aspects*

It is nowhere more clear than in the case of materials information, that no one country has a 'corner' on the key information nor on the optimal systems design for storing, manipulating and accessing it. For precisely this reason international cooperation is to be encouraged in every way. Existing international organizations such as CODATA (Committee on Data of the International Council of Scientific Unions) and ISO (International Organization for Standardization) have important roles to play as do the Commission of the European Communities and various bilateral projects.

5.6. *Concluding comment*

This paper has ranged over a number of interrelated themes: materials science, information technology, and engineering. It is only through the enlightened and assiduous application of understanding of all three that the 'promise of advanced materials' will be realized.

The authors are indebted to J. G. Kaufman, J. L. McCarthy and C. J. M. Northrup, Jr, for helpful critical reviews of the paper in draft form.

REFERENCES

AGORA 1983 *Information on a changing World*, vol. 5. Rome: Intergovernmental Bureau of Informatics.
Ambler, E. 1985 *ASTM Standardization News*, p. 46. Philadelphia: ASTM.
Brown, W. F., Jr, (ed.) 1983 *NMAB-NRC report NMAB*-405. Washington: National Academy Press.
Bullock, E., Kröckel, H. & Van de Voorde, M. 1986 In *Proc. CODATA Workshop, Schluchsee, Germany*.
CEC 1983 *First demonstrative report on the high temperature materials data bank of JRC*, EUR 8817 ENfs. Luxembourg: CEC.
Dathe, G. 1985 In *Proc. 9th Int. CODATA Conf., Jerusalem, Israel*, pp. 233–240. New York: Elsevier.
Dixon, J. R. & Simmons, M. K. 1983 *Computers in mechanical engineering*, p. 10. New York: Springer Verlag.
Fattori, G., Krefeld, R., Kröckel, H. & Maurandy, C. 1985 In *Proc. 9th Int. CODATA Conf., Jerusalem, Israel*, pp. 251–254. New York: Elsevier.
Fattori, G. & Krefeld, R. 1987 In *Proc. 10th Int. CODATA Conf., Ottawa*. (In the press.)
Graham, J. A. *et al.* 1980 *Mechanical properties data for metals and alloys, NDAB-NRC*. Washington: National Academy Press.
Grattidge, W., Westbrook, J. H., Northrup, C. Jr, McCarthy, J. and Rumble, J. Jr 1986 *Materials information for science and technology* (*MIST*) *Project Overview*. Gaithersburg, Maryland: NBS.
Guile, B. R. (ed.) 1985 *Information technologies and social transformation*. Washington: National Academy Press.
Hampel, V. E., Bollinger, W. A., Gaynor, C. A. & Oldani, J. J. 1984 UCRL-90276, University of California, Livermore, California.
Hayes-Roth, F., Waterman, D. A. & Lenot, D. B. (eds) 1983 *Building expert systems*. Reading, Massachusetts: Addison Wesley.
Heppenheimer, T. A. 1985 *High technology*, **5**, 62.
Joy, W. & Gage, J. 1985 *Science, Wash.* **228**, 467.
Kaufman, J. G. (ed.) 1986 *Materials data for the petrochemical industry*. American Petroleum Institute.
Kaufman, J. G. 1986*a* In *ASTM Standardization News*, p. 28.
Kaufman, J. G. 1986*b* In *Chemical Engineering Data Sources*. (AIChE Symposium Series 247.)
Klein, A. J. 1985 *Advd. Mater. Processes* **2**, 43.
Klein, A. J. 1986*a* *Advd. Mater. Processes* **4**, 20.
Klein, A. J. 1986*b* *Advd. Mater. Processes* **2**, p. 33.
Kröckel, H., Reynard, K. & Steven, G. (eds) 1985 *Factual Material Data Banks* (CEC Workshop – JRC Petten), EUR 9768 EN. Luxembourg: CEC.
Kröckel, H. & Steven, G. 1986 In *Proc. 10th Int. CODATA Conf., Ottawa, Canada*. Amsterdam: Elsevier.
Kröckel, H. & Steven, G. 1987 In *Materials property data – applications and access* (ed. J. G. Kaufman), MPD vol. 1–PVP vol. 3, pp. 175–182. New York: ASME. (In the press.)
McCarthy, J. L. 1982 In *Proc. 8th Int. Conf. on Very Large Data Bases, Mexico City*, pp. 234–243.

Naisbitt, J. 1982 *Megatrends, ten new directions transforming our lives*. New York: Warner Books.
NBS 1984 A workshop held at the national bureau of standards, NBSIR84-2907.
Northrup, C. J. M., Jr, McCarthy, J. L., Westbrook, J. H. & Grattidge, W. 1987 In *Materials property data: applications and access*. ASME. (In the press.)
Oren, T. & Kildall, G. A. 1986 *IEEE Spectrum*, p. 49.
Pin-Shan Chen, P. 1986 *IEEE Spectrum*, p. 44.
Quinn, G. D. & Baratta, F. 1985 *Advd. Mater. Processes*. **4**, 31.
Reynard, K. W. 1986 *Metal. Mater.*, **2**, 147–149.
Rumble, J. R. (ed.) 1986 *Tribology data systems*. U.S. Dept of Commerce
Rumble, J. R. & Northrup, C. J. M. Jr, (eds) 1986 *A workshop for ground vehicle engineering*. Society of Automotive Engineers.
Rumble, J. R. & Westbrook, J. H. (eds) 1985 *A workshop for the nuclear power industry*. NBS SP 689.
Salzman, R. M. 1985 *Computer Graphic* **9**, 435–439.
Sargent, P. 1985 Metal. Mater., **1**, 540.
Schwarz, S., Watson, D. G. & Alvfelt, O. (eds) 1985 *Non-bibliographic data bases in science and technology*. Miami: ICSU Press.
Shoshani, A., Oklen, F. & Wong, H. K. T. 1985 In *Proc. 9th Int. CODATA Conf., Jerusalem, Israel*. New York: Elsevier.
Sowizral, H. 1985 *A. Rev. Inf. Sci. Tech.* **20**, 179–199.
Swindells, N. & Swindells, R. J. 1985 *Metal. Mater.* **1**, 301–304.
Toffler, A. 1980 *The third wave*. New York: William Morrow and Co.
Weiss, V. & Aha, D. W. 1984 *SAMPE Proceedings* **29**, 506.
Westbrook, J. H. 1982 *A study for the metal properties council.*
Westbrook, J. H. 1983 In AGARD Lecture Series, 130, pp. 9/1–9/9. Neuilly-sur-Seine: Advisory Group for Aerospace Research and Development.
Westbrook, J. H. 1985*a* In *Proc. 9th Int. CODATA Conf., Jerusalem, Israel*. New York: Elsevier.
Westbrook, J. H. 1985*b* *NBS special publication 702.*
Westbrook, J. H., Behrens, H., Dathe, G. & Iwata, S. (eds) 1986 In *Proc. CODATA Workshop, Schlüchsee, Germany.*
Westbrook, J. H. & McCreight, L. (eds) 1986 *Computerised materials property and design data for aerospace technology.* AIAA. (In the press.)
Westbrook, J. H. & Rumble, J. R. (eds) 1982 In *Proc. Materials Data Workshop, Fairfield Glade, Tennessee.*
Williams, F. 1982 *The communications revolution.* Beverly Hills, California: Sage Publications.

Discussion

J. F. Barnes (*R&D Establishments and Research, Ministry of Defence, London, U.K.*). May I say first how much I enjoyed listening to what Dr Westbrook had to say? I ask for his comments on the potential implications for industrial structure. It seems to me, that when complex composite components have to be manufactured, the traditional pattern where, for example, an aeroengine manufacturer would seek supplies from several sources for his components will cease. The supplier will have to be identified at an early stage of the design process and will have to be associated with all aspects of experimental manufacture if he is to produce components that meet the requirements of the designer. In consequence, the overall manufacturing process may tend to become much more integrated and the practice of having suppliers in competition with each other may die or diminish. Do you agree?

R. W. Cahn (*Department of Metallurgy and Materials Science, University of Cambridge, U.K.*). Dr Westbrook mentioned the importance of achieving an international standardization of the designation of alloys and other materials, to facilitate the construction of useful computer databases. Considering, however, the strength of national pride in such matters, might it not be more profitable to exploit the speed of computer interrogation by constructing tables of international equivalents and automatically consulting these before a computer has to throw up its metaphorical hands in mystified despair?

M. O. W. **Richardson** (*Department of Materials Engineering and Design, Loughborough University of Technology, U.K.*). It seems to me that additional to the need for expert materials systems that are 'user friendly' there is a need for 'friendly expert users' to operate the expert systems. In other words the complexities of modern composite materials are so great that we shall require the universities to produce *more* materials engineers and scientists to operate these systems effectively. We are asking for trouble if we think that easy access to data banks will automatically enable even the best mechanical engineers to have a deeper understanding of the materials they are using, for example, how many engineers know about the interfacial and interphase problems associated with composite materials and how this may affect generated data?

N. **Swindells** (*Matsel Systems Ltd, Mount Pleasant, Liverpool, U.K.*). Dr Hondros raised the important requirement for standardization of databases so that users would not be faced with a great diversity of systems. I can report that efforts to overcome this problem are being made within the EEC as a result of programmes initiated by the Directorate General XIII/B of the Commission of the European Communities. An experimental programme of collaboration between eleven producers of materials information systems in four countries has produced the first draft of proposed standards for the operation and presentation of materials property information systems. These standards refer to four levels in the information systems: access, host operations, system operations, contents. They will form a framework for the operation of a pilot programme for an integrated organization of materials property information systems called the Materials Databanks Demonstrator Programme, which is expected to be operational early in 1988.

The discussions that lie behind the development of these standards are evidence of a strong commitment to collaboration in these matters at an international level within the EEC and similar efforts are also being made by international collaboration over a wider range.

J. H. **Westbrook and** H. **Kröckel**. We would like to thank all the contributors to this discussion for their interest and comments. In reply to Mr Barnes, we would agree that developments in composites, as well as in other advanced materials, are likely to alter traditional relations between manufacturer and materials supplier. We also agree with Dr Richardson that even the friendliest and most expert computerized information systems are unlikely to put the materials scientist or engineer out of work. His talents will be required more than ever, both in building and improving these systems and in exploiting the more sophisticated materials 'designs' the systems will project. Professor Cahn's suggestion of a built-in cross-reference to various international equivalents for materials designations is indeed being incorporated in several of the information systems now being designed and built. Such a feature will be helpful but will not lessen the benefits of standardization. Various American, European and world-wide efforts mentioned in our paper show the critical importance of this standardization issue. Dr Swindells's contribution commendably supplements this by describing the joint development under his coordination of a CEC code of practice for the operation of a materials databanks pilot network in the European Community.