NBSIR 84-2907

Report of a Workshop

The Effect of Computers on the Generation and Use of Technical Data

National Bureau of Standards
Gaithersburg, MD
March 19 - 20, 1984

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
Office of Standard Reference Data
Gaithersburg, MD 20899

June 1984

UNITED STATES DEPARTMENT OF COMMERCE
National Bureau of Standards
Washington, D.C. 20234

August 24, 1984

MEMORANDUM FOR Attendees at the Workshop on the Effect of Computers on the Generation and Use of Technical Data

From: David R. Lide, Jr.
Director, Standard Reference Data

The Report of the Workshop is attached. I hope you will find this of interest and would appreciate any comments or suggestions for follow-up action.

I might call your attention to Appendix III, an annotated bibliography of studies and reports dealing with data needs.

Let me thank you again for your participation in the Workshop. Your contributions were extremely helpful to us.

Attachment

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David R. Lide, Jr., Editor

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PREFACE

This report is a summary of the Workshop on the Effect of Computers on the Generation and Use of Technical Data, which was held at the National Bureau of Standards on March 19-20, 1984. It includes synopses of the talks presented at the Workshop and reports from the working panels which met to discuss specific topics. An Executive Summary is also included.

The synopses were prepared by the staff of the Office of Standard Reference Data, viz.:

Sherman P. Fivozinsky
Bettijoyce B. Molino
John R. Rumble, Jr.
Howard J. White, Jr.

Credit is also due to the chairmen and secretaries of the working panels, as well as to all who participated in the Workshop.

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EXECUTIVE SUMMARY

The National Bureau of Standards held a Workshop on the Effect of Computers on the Generation and Use of Technical Data on March 19-20, 1984. The Workshop addressed changes in the generation, dissemination, and use patterns of scientific and technical data which are occurring as a result of the widespread introduction of computers. The principal conclusions of the Workshop are summarized here.

- Comprehensive, reliable data bases covering physical, chemical, and mechanical properties of substances and materials form an essential resource for U. S. industry. Such data play a key role in research, development, engineering design, and process control.

- Modern computer technology has already had a profound effect on the way engineers do their work and on the way data are analyzed and organized. CAD/CAM techniques have proved their value in many industries, and computer graphics has become a powerful tool. However, the integration of data bases and design/manufacturing programs is still at a relatively primitive stage.

- The use of computer/telecommunication techniques for transfer of data from data bases to the user's programs has several advantages:

  - The best data sources can be located more reliably and quickly.

  - Multidimensional searches, multiple access paths, and searches for materials with given properties, which are not feasible with conventional printed tables, can be exploited.

  - Data bases can be updated in a more timely fashion than is feasible with print media.

  - Automated transfer of data from data base to application program is more economic and less error-prone.

- There are no significant technical barriers to achieving the above advantages, but progress is currently limited by several factors:

  - Very few validated machine-readable data bases exist with broad enough coverage to meet the requirements of the relevant technical community.

  - Scientific data, with their wide range of formats, impose special demands on data base management systems.

  - Little standardization has been achieved in the terminology for materials, chemical substances, properties, uncertainty indicators, and other data elements.

  - The interface between existing data dissemination systems and the working scientist or engineer is generally inefficient and hard to use.

- o Many organizations can and should play a role in overcoming these barriers and realizing the potential benefits of computer-based data dissemination systems. These include scientific and technical societies, industrial trade associations, the commercial information industry, and Government agencies.

- o There are major needs, documented in this report for a series of technical areas, for comprehensive, validated data bases in a computer-searchable and transferable form. A very promising avenue for supplying these data bases lies in the development of predictive models which provide the user with the desired property data for any specified set of environmental parameters. The improved scientific understanding of the relation between macroscopic properties and microstructure, together with the power of modern computers, has opened exciting possibilities for developing such predictive models.

- o The National Bureau of Standards has several well-recognized roles to play in these endeavors, including:

  - Preparation of evaluated data bases and development of predictive models.

  - Leadership in the establishment of validation procedures and quality control of data bases.

  - Leadership in the development of format and interface standards and of data base management systems which will allow providers and users of technical data to communicate effectively.

  - Helping to bring all of the involved institutions together to work cooperatively on problems of common interest.

INTRODUCTION

Numerous studies have demonstrated the importance of reliable technical data in research, development, and engineering design. Pressures on U. S. industry, especially in the last 10 years, have highlighted the need for careful design of plants and processes so as to optimize their performance and avoid costly, and in some cases catastrophic, failures. Accurate data on physical, chemical, and mechanical properties of substances and materials are a key element in the design process. Moreover, these studies have shown that timeliness in the availability of data is essential, because the complex, multi-step design procedures inherent to modern technology do not permit delays to locate data that are not at hand.

Under the Standard Reference Data Act of 1968 the National Bureau of Standards was given the central responsibility for promoting and coordinating U. S. data activities. NBS has conducted a program to compile and evaluate data and to publish the results in a form accessible to the user communities. The approach followed has involved retrieval of data published in the scientific literature, critical evaluation of these data with the aid of methodology developed for each scientific area, and preparation of tables of recommended values. The results have been published in handbook or journal article format. In carrying out this program, NBS has involved not only its in-house experts but also scientists in universities, industry, and other government laboratories.

The rapid advance in computer power in the last 10 years has set in motion some major changes in the way technical data are generated, stored, disseminated, and used. It is possible with modern computers to correlate or fit large amounts of experimental data from diverse sources which are related through a verified theoretical framework. The resulting physical model provides not only a means of checking for inconsistencies in the original measurements but also may have a valuable predictive capability. Furthermore, computer-readable numerical data bases are now coming into use as an alternative to printed compilations; the retrieval capabilities of computerized data systems offer significant advantages over printed compilations. Finally, the users of technical data, especially at the engineering level, are making increasing use of computers for design, manufacturing, and process control.

This Workshop brought together key individuals who are concerned with the generation, dissemination, and use of data. Its objective was to discuss the changing use patterns and assess the resources available for meeting these new needs. A particular goal of the Workshop was to identify the barriers that must be overcome in order to realize the full benefits of this new computer and telecommunications technology.

The format of the Workshop included general talks on the use of computers in design and manufacturing and more specific talks on needs for selected classes of physical, chemical, and materials data. Ten working panels were set up to discuss the issues in the context of the most important types of technical data. This report presents synopses of the talks which were presented and recommendations from the working panels.

SYNOPSES OF GENERAL TALKS

The Federal Role in Stimulating Industrial Competitiveness

John P. McTague
Deputy Director, Office of Science and Technology Policy
Executive Office of the President

There are two aspects to the activity of data evaluation and the development of materials properties data bases. One is the scientific effort of producing reliable data bases, and the other is the use of these data bases in industrial or technological applications. The second aspect is highly relevant to the Federal role in stimulating industrial competitiveness.

The U. S. position in the international trade community is bad, and it is deteriorating. In 1980 alone the trade deficit was in excess of 24 billion dollars. However, in high technology trade we had a surplus of 30 billion dollars, in contrast to a deficit of about 55 billion dollars in other areas. The need to promote high technology in industry as a whole is clear.

We do well in such fields as computers, office equipment, plastics, aircraft, medical equipment, drugs, etc. In fact we are preeminent in the world in these fields. Each of these industries has a high level of scientific and engineering skill and a high percentage of research and development relative to sales. As far as a balance of trade is concerned, it appears that a high level of innovation is necessary as well as a rapid rate of technological development.

Innovation and creativity have always played an important role in this country. Our continuing scientific creativity is demonstrated by the large share of Nobel Prizes captured by Americans. What we must do is find ways to provide rapid technology transfer of these new ideas to industry. We need to set goals for contributing to this new technology, communicate these goals, and remove impediments to translating creativity into new products.

The Federal role in this process is exemplified by three rules:

1. If somebody else has the motivation to do it, they will do it better than the Government.

2. When benefits are too long range for the private sector (like basic research), the Government should get involved.

3. The Government should be involved in those areas (like defense) where it is the prime user of R&D results.

The steel and machine tool industries are examples of major trouble spots in the American economy. There is a great need for automation of steel-producing processes, which are still almost completely manual. This is a perfect example where standard reference data should play a role. Thermodynamic properties and chemical rate data, if available through a computer system, would help continuously monitor the processes involved. There is a great opportunity here for increased effficiency. At the present time 45 percent of the price of steel is labor. This is a clear example of where high technology, computerization, and standard reference data could lead to more modern and efficient processes.

The problem is to get new technology into these mature non-high-tech industries. The Government's role is not to do the job, but rather to break down barriers between these industries and the institutions which could enter a partnership to help solve the problems. There are people in the National Laboratories, for example, who know a great deal about processes used in the steel industry. The Government should serve as a marriage broker for such partnerships involving universities, technical societies, and other institutions.

In the long run the Government must promote the creation of good talent through the support of university research and the training of students. NSF is now supporting integrated engineering research centers at universities to look at such things as computer-assisted manufacturing and other innovative approaches to industrial problems. In all of these new approaches to promoting the Nation's technological health, there will be increasing requirements for dependable and up-to-date data bases on the properties of materials.

Computerization of the Design/Production Cycle

Michael Wozny
Director, Center for Interactive Computer Graphics
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Computers are changing, in a very fundamental way, the way industry operates. Manufacturing is becoming data-driven; that is, it is moving away from being controlled by the processes themselves toward a situation where data controls the whole operation. In this move towards automation, many processes are becoming more transparent to the human operators, which means that, as we lose some of the control, it is necessary for the data to be more timely and more reliable. This increased need for timely, reliable data is one of the issues of this workshop. A second issue concerns the role of computer graphics in data handling. As computer graphics become more sophisticated, the means of presenting data must be reconsidered.

The data flow in a large design/production environment follows a well-understood pattern. After receiving production demand data from marketing and sales, engineering creates product definition data to be supplied to the manufacturing environments; this, in turn, creates for the planning phases both process definition data and scheduling and control data. These data form input to the actual physical processes for manufacture of the final product. The key areas are, therefore, the product definition, the process definition, and scheduling and control. In an automated manufacturing environment all data are processed through interactions of graphic displays under computer control as the product is defined in the geometric modeling sense. The models create and run processes and software programs to drive the computers in the scheduling and control process. The whole system is tightly integrated, with a high demand on the quality of technical data used. The goal of such a system is to automate completely the creation, analysis, transmission, and management of data, such that control of the physical processes is driven by the data. Once again, these data are becoming more important in American industry, and we are seeing scientists making careers of controlling data rather than products.

The computerization of the design/production cycle began in the early 1960's with the automation of drafting; at this time the computer knew only how to draw lines, make connections, and select orientations. That advance, along with the automation of machine tool operations, led to increases in productivity because the machines could keep track of all the automated parts. Problems arose, however, with human-computer interfaces, an area which still presents major problems.

The resulting increase in productivity launched the turnkey industry, which began in the late 1960's or early 1970's but did not gain full momentum until 1975-1977. At that time there were many turnkey companies which inserted coding into computer systems purchased from someone else, leading to an end product on which the designer could turn a key and begin drafting. There was no standardization and each organization, once trained on a specific device, was resistant to change. These turnkey systems did drawings--nothing more--and it was not until around 1980 that things began to change.

Future CAD/CAM directions are now becoming clearer. CAD will grow in directions other than drafting and will be more than a tool for artwork. More important, there will be a sharing of information among the various parts of the production process. Automation will permit the production cycle to use computers from the design and analysis stage right through manufacturing, test, and interproduct support.

This approach is not without problems, however. Depending on the size of the company, there can be any number of computer systems or any number of data bases, which creates data format problems. An example of a successful solution of one such standardization problem is the ANSI adoption of the Initial Graphics Exchange Specifications (IGES). With NBS exerting a leadership role, this standard was quickly adopted by ANSI, and many vendors are complying in integrating it into industry.

Shared information in the drafting, design, and development phases must now be transferred into the planning and tooling phases. The factory of the future will be controlled by CAD through manufacturing, planning, and control systems and by CAM through execution in a robotics environment.

One of the fastest growing areas in the use of computers in engineering is expert systems. An expert system is, simply, a body of knowledge with mechanisms to interpret this knowledge. From a developed set of rules, by checking facts against these rules, other facts and other rules can be inferred. There are many facets to the development of expert systems such as acquiring knowledge, establishing a rule base, dealing with uncertainties and inconsistencies, and allowing for a changing system where the rules may change.

Today there are still many things related to design automation that we do not know how to do. One cannot deform solids arbitrarily; tolerances are not easily dealt with; models cannot be automatically analyzed to a predefined accuracy; models cannot drive execution and planning functions; there is no good language to control robots; and there is not enough information on sensors. There are no optimizing algorithms to take large complexes of multimachine manufacturing cells and schedule and optimize operations.

Computer graphics, a subset of this CAD/CAM environment, is increasing productivity by providing a better interface between people and data. It permits ease in visualizing, manipulating, and understanding the data. Graphics provides a good means of presentation, especially for technical data. Powerful graphics capabilities exist and are rapidly moving into the commercial world, where they will be able to portray and handle data in the future.

Materials Data for the Factory of the Future

Michael J. Jefferies
R&D Manager, Engineering Physics Laboratories
General Electric Company

The factory of the future can be discussed in terms of four phases of the production cycle:

- Computer-aided design (CAD)
- Computer-aided engineering analysis (CAE)
- Computer-aided manufacturing (CAM)
- Computer-aided testing (CAT)

Data bases and communications, the technologies of storing and moving information, form the centerpiece tying this factory of the future together. Every part of the production cycle needs data of various types, including materials data.

Computer-aided testing is exemplified by a GE system called TMGR, which comprises computer software for managing tests of turbines and compressors. It sets up test conditions, takes data, and does real-time calculations on efficiency. The materials property data needed are the thermodynamic properties of the working gas.

Generally we find that CAT does not generate demand for new kinds of materials data. However, there is a need for new ways of data access so as to insure that the properties data used for testing are the same as those used for design. This need for access to consistent data by different production functions is a general trend in advanced factory systems. A computerized materials data base can accomplish this if it is properly designed.

An example of computer-aided manufacturing is provided by work being done to automate gas tungsten arc welding. Expert human welders usually make good welds by choosing an arc current, then adapting the torch speed and wire feed rate based on the appearance of the weld and their past welding experience. The automated system uses a different approach. Instead of setting welding parameters by trial and error, they are determined, at least in part, by referring to the fundamental materials properties governing the process.

These properties include thermal conductivity, heat capacity, latent heat of fusion, density, and surface tension. The properties are used to calculate the shape and depth of the weld puddle for a given set of welding parameters. The results are used in turn in an adaptive control algorithm which interprets video images to adjust the current, torch speed, and wire feed during the actual welding process. The system has already demonstrated weld quality better than that of human experts, and with much higher productivity.

A second example of CAM concerns injection molding of plastics and die casting of metals. Here the requirement is to fill the mold completely, and also to control the positions of knit lines which occur where different flow channels meet. It is desirable to cool the part so that it can be removed from the mold as rapidly as possible. At the same time the temperature swing of the mold must be kept to a minimum for long mold life. Computers have made it possible to start with a fundamental understanding of the molding process in order to design better molds, and optimize process temperatures, pressures, and times. Examples of data needs are viscosity as a function of temperature, heat capacity; thermal conductivity; heat of fusion; compressibility; and thermal expansion. Data for some materials are available, but for other materials, including plastics and blends, more and better data are badly needed.

These two examples of advanced CAM technology illustrate a need for new materials data -- data describing properties under processing conditions. In the past, processing parameters were determined empirically. However, computer control requires a more fundamental description of processing, and this requires data often quite different from that which characterizes the performance conditions. Access to process-related materials data is usually not required in real-time but rather during the design of the processing procedure.

The object of computer-aided engineering analysis is to predict product behavior while keeping expensive prototype tests to a minimum. An example of CAE is electromagnetic analysis of motor designs. The designer makes choices about shapes for laminations, type and amount of electrical conductor, and type of magnetic materials. The computer then does a two-dimensional, nonlinear electromagnetic analysis. The results are as accurate as the materials data that are used. The data include electrical conductivities and temperature-dependent magnetic hysteresis curves. For motor analyses, the data are reasonably good. For other analyses however, like nonlinear time-dependent structural behavior of plastic parts, there are needs for new and better quality properties data.

CAE programs today are usually very particular about how they accept materials data. Often these data must be hand-fed to the programs by users familiar with the format required. In the future, when large numbers of users want to do analyses with a choice of hundreds or thousands of different materials, direct computer access to materials properties data bases will be essential. These will have to be organized in such a way that an analysis program can call for needed properties without having to know the details of the data base structure.

The last step through the factory of the future brings us to computer-aided design, the use of computers to develop design concepts. The CAD tools of today primarily help the designer visualize a concept, for example by representing two- and three-dimensional geometry. CAD is not usually associated with materials selection, but a computer system could consider operating conditions, performance, and cost, and then suggest appropriate materials. Such a system would need access to a wide range of information on materials, including non-quantitative heuristic data.

To accomplish this we need "intelligent" data bases, that is, systems capable of reasoning deeply about the queries with which they are presented. Such data bases must be able to retrieve items according to quite general criteria not directly tied to a particular data base organization. They should be capable of dealing with statements such as "find all coating materials suitable for gear teeth operating in an abrasive environment."

In cases where the user cannot even frame the right question, an expert systems approach might be best. Expert systems capture in a computer program the domain-specific knowledge of one or more human experts. The program can then perform like an expert in solving problems in that domain. The challenge is to represent and manipulate the expert knowledge, which is usually only partly in the form of numerical property values. Often it consists of empirical associations and logical assertions such as "copper-nickel alloys are generally suitable for marine applications." Useful materials expert systems should be possible with a reasonable extension of today's technology.

In summary, the technical data community and the National Bureau of Standards can have the greatest impact on materials data needs for the future factory through the following activities:

- The top priority is the exploration of opportunities for expert systems. This could be a valuable future tool for engineering design, and the technology here is ripe for exploration. The utlimate payoff could be very large.

- Second, a major effort should be focused on materials property data at processing conditions.

- Third, the time is right to develop data base standards for format-independent computer access methods so design analysis programs and other computerized systems in factories can talk to materials data bases.

Challenges for the Technical Data Community

Ernest Ambler
Director, National Bureau of Standards

Where it has not happened already, the computer will soon become a central tool for scientists and engineers in all fields of activity. The changing practices introduced by the increased use of computers will affect all of us. Engineers must learn new ways to access data and must become more sensitive to the quality of data, because the penalties of using bad data can be very costly. The organizations that disseminate technical data, both professional societies and the commercial sector, are already beginning to make the transition from traditional handbooks and journals to computer-based formats. Finally, the technological agencies of the Federal Government, including the National Bureau of Standards, must be aware of the effect of these new patterns of data use on the generation and organization of data pertinent to their missions.

In our pluralistic society the various institutions with a stake in scientific and technical information find their respective roles through a process of consensus and competition, rather than centralized planning. None of us expect this tradition to change, but it leads to a potential danger that new information delivery systems may be created in a helter-skelter way. Furthermore, an extra effort might be required to make them compatible with the design programs being developed by the end users of the data. Each of the organizations involved in data base generation, dissemination, and use should recognize that its own self-interest dictates a need for coordination and standardization.

Among the barriers which stand in the way of an orderly development of data systems that will meet the needs of users are, first of all, the creation of validated data bases which can provide the answers to queries from diverse and unpredictable sources. A second barrier is the special requirements which scientific data, with their wide range of formats, impose on data base management systems. Another barrier lies in the need for standard terminology for materials, chemical substances, properties, uncertainty indicators, and other data elements. Finally, the interface between a data dissemination system and the working scientist or engineer must be made easy to use.

The National Bureau of Standards can play two roles in overcoming these barriers. First, we can address the problem of building the evaluated data bases; this is a traditional NBS function, one which Congress has specifically mandated as an NBS responsibility. Second, we can serve as the broker in bringing about the computer compatibility and standardization required to disseminate the data effectively.

Our approach to producing data bases has changed in a significant way over the last two decades. It has become feasible to extend the scope of directly-measured experimental data by the use of physical models that describe the relation between the property in question and the parameters on which it depends - the microstructure of the substance or material and the temperature, pressure, and other environmental factors. The opportunities for doing this have greatly expanded because of two developments: an improved scientific understanding of the quantitative relationship between macroscopic properties and microstructure, and the power of modern computers which make it possible to carry out the complex calculations necessary to obtain usable numerical results from the mathematical models. Thus, in many cases, we can now use a limited set of experimental data coupled with the appropriate theoretical framework to develop a model that permits prediction of property values outside the range of actual experimental study. This is a very powerful approach, one that provides a comprehensive algorithm which will give a user the specific data he needs, regardless of whether those data have actually been measured in the laboratory.

The National Bureau of Standards is prepared to work with all interested parties to overcome the compatibility and standardization problems. Recent examples of NBS activities of this type include the development of computer network protocols and the Initial Graphics Exchange Specifications (IGES), which allows CAD systems from different manufacturers to talk to each other. NBS has a long tradition of cooperation with professional scientific and engineering societies and industrial trade associations, as well as effective links to the pertinent international organizations.

With the advice and help of all concerned institutions, NBS is prepared to provide the leadership that will permit the private and Government sectors to work together in accomplishing the efficient production, dissemination, and use of technical data.

NEEDS AND RESOURCES IN SELECTED TECHNICAL AREAS

Three areas were chosen for a more detailed examination of the present and anticipated needs for reliable data bases and the resources for meeting these needs. Each area was discussed first by an industry representative, who gave the users' perspective, and then by an NBS representative who described existing resources and oulined plans for the future. These talks are summarized here.

Fluid Properties and Thermochemical Data

David W. H. Roth, Jr.
Director, Office of Science and Technology
Allied Corporation

Neil Olien
Chief, Chemical Engineering Science Division
National Bureau of Standards

In the chemical and related industries underdesign of a unit in a production process will surely lead to costly retrofits and production time lost. A design engineer faced with questionable data in a design calculation will accordingly add an overdesign safety factor. The consequences of doing this are not trivial. Capital costs will be escalated and in an extreme case a sound investment opportunity may be abandoned in pre-project analysis. There may be a mismatch of unit processes leading to increased operating costs or worse-than-specification performance because the overdesigned unit is forced to operate out of its optimum range of performance.

Lack of precise design data and reliable well-understood correlation and prediction tools has cost the chemical process and petrochemical industries billions of dollars, has resulted in catastrophic failures costing lives, and has resulted in environmental traumas which in many cases have persisted for decades. In the chemical and related industries with annual sales of $150 billion, operating costs of $125 billion, and an annual capital investment of $10 billion, the availability of more precise data and more reliable and better understood data-correlation tools and models, used in currently available computer-based modeling programs, would reduce annual capital investment and operating costs by 5 percent, for annual savings of over $7 billion. Current data activities in the U. S. have been estimated as $7 million in 1977 and $9.5 million in 1982, about 0.01 percent of the estimated potential benefits. An order of magnitude increase in data efforts is warranted.

Industry has increased its own efforts recently through the establishment of the Design Institute for Physical Property Data (DIPPR). The current program of DIPPR will represent a direct investment of $2.25 million which will be increased by an estimated $3-4 million by contributions in kind from participating industrial data specialists.

Current trends in industry are away from large plants for commodity chemicals and toward smaller plants for specialty chemicals with demanding requirements for product purity, composition control, and quality. More understanding at the micro level will be required to produce these increasingly complex and sophisticated products and to design plants using the large-scale process-integration design calculations which are currently being developed.

Better prediction techniques are needed for all properties of mixtures over a wide range of conditions. More powerful and reliable nonlinear regression techniques are needed, as well as standardization of data bases and prediction techniques to permit transportability and loading into various design codes and process simulators. Accurate new measurements on key compounds and mixtures are needed and existing correlations and estimation techniques must be reviewed in the light of the new data.

The fulfillment of these requirements and the creation of the computer tools needed will be a technical task of high order. Generalized predictive techniques will be needed which provide property data of standard-reference-data accuracy. To bring such techniques into being will require a coordinated program of theory, experiment, and data evaluation all focused on the development of accurate wide-range correlations and predictive techniques. A major function will be the validation of the performance of predictive techniques. It is essential that the user of predictive techniques receive with the computer package factual information on its performance and limitations.

Techniques must be developed for highly polar substances, substances at high temperature and pressure, and substances containing a large and variable number of components.

Starts have been made on many of these needs and promising new techniques are available in some cases. However, a long-term scientific and technical program will be needed to meet the listed requirements. In addition, much software standardization must be completed to meet requirements for transportability and ease of use.

NBS should play a leadership role in coordinating the efforts of the industrial and professional groups in the United States and cooperating with on-going efforts in other countries.

Atomic, Molecular, and Nuclear Data

James J. Wynne
Manager, Laser Physics and Chemistry
Watson Research Center
IBM

Wolfgang Wiese
Chief, Atomic and Plasma Radiation Division
National Bureau of Standards

Atomic and molecular data have played, and continue to play, a key role in many aspects of science and technology. There was a direct connection between the development of quantum theory and the availability of a knowledge-base (data base) of spectroscopic information. The importance of atomic and molecular spectroscopic data, such as energy levels and transition probabilities, to the development of lasers illustrated the applicability of such data to technology. The present industrial development of ultraviolet laser techniques demonstrates the continuing requirements for new atomic and molecular data pertinent to these spectral regions and emphasizes the direct relationship between the availability of these data and the possibility of technological success. For example, the shortest wavelength commercially available cw laser is the He-Cd laser at 325 nm. In seeking shorter wavelength lasers, high stages of atomic ionization must be accessed. In many instances the atomic parameters are not yet known for the species that could become the best laser candidates.

Atomic data are crucial to magnetic fusion reactor development for future electric power generation. Tokamak-type fusion plasmas require atomic data both for diagnostic studies of the behavior of these plasmas and in the design of the overall systems. There are particular needs for spectroscopic data on very highly ionized species of the impurity elements that tend to poison the plasma and prevent it from attaining the required operating temperature.

In addition, models of the ionization distribution of an impurity element from the walls to the center of the plasma can be constructed from ionization rates and radiative and dielectronic recombination rates using densities and temperatures derived from diagnostics. Comparison of the models with line intensity distributions can be used to study transport of ions in the plasma. The electron and ion temperatures in a plasma can be quite different. Forbidden lines at ultraviolet wavelengths are advantageous for investigation of the ion temperature through measurement of the Doppler width.

The next generation plasma devices now under design, which are expected to attain "break-even" or possibly "net energy gain" conditions, will require even more esoteric data. These data will have an enormous economic impact since each new device will cost up to one billion dollars. The availability of good data needed for the analysis and monitoring of high-temperature plasmas and for the evaluation of power losses by radiation will enable considerable cost savings in the design process. Other new developments, such as nuclear driven x-ray lasers, will require the use of similar data on highly ionized atoms.

The successful implementation of new techniques for surface studies and microelectronic circuit fabrication depends on the availability of atomic spectroscopic data. The etching rate in the production of microcircuitry is strongly enhanced because various species in the plasma are produced in excited electronic states, leading to increased chemical reactivity. The monitoring of this process by laser spectroscopy will depend on data not currently available covering species such as carbon, fluorine, aluminum, silicon, chlorine, titanium, copper, and their ions (as well as on molecules and radicals).

Parameters such as energy levels, absorption cross sections, isotope splittings, hyperfine structure, lifetimes and branching ratios, and field and collisional ionization rates from Rydberg states are vital to the design of processes for isotope enrichment and resonance ionization mass spectrometry, which is becoming an increasingly important tool of the analytical chemist.

A recent report on Current Trends in Atomic Spectroscopy, prepared by the NAS/NRC Committee on Line Spectra of the Elements, illustrates further the detailed areas of atomic data evaluation where new work needs to be carried out.

Data centers at NBS contribute strongly to the atomic and molecular data evaluation effort. Another important resource is the fusion data center at Oak Ridge National Laboratory. The U. S. Nuclear Data Network, which is primarily supported by the Department of Energy, covers data on neutron cross sections, nuclear structure, and reactions. International coordination of nuclear and atomic data activities is provided by the International Atomic Energy Agency in Vienna.

Predictive techniques will be very useful in supplying atomic and molecular data. Extrapolation along isoelectronic sequences and use of quantum defect theory have already proved their value. There are opportunities for developing more sophisticated prediction schemes which will reduce the need for new laboratory measurements. Advances in the theory and in the techniques for ab initio computation of atomic and molecular properties open the door to a productive interplay of experimental measurement, data evaluation, and model development which will be able to supply the data needed at both the scientific and technological level.

Materials Performance Data

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Chief, Metallurgy Division
National Bureau of Standards

In real design problems, the required materials data usually cover a diversity of properties. For example, to design a superconducting generator, needed material data might include:

- o Properties of structural materials at cryogenic temperatures
- o Electric properties of dielectrics
- o Mechanical properties of structural composites
- o Superconducting properties
- o Magnetic properties of materials
- o Thermal properties of cryogens

However, through all these data and their use run three fundamental concerns, namely, reliability/evaluation, access/dissemination, and prediction/modeling.

Reliability/Evaluation

From the viewpoint of a materials data user, reliability of technical data is a most important issue. If data are reliable, they are acceptable as design values. If not, overdesign must be practiced, and overdesign is expensive. Consequently, evaluation of materials data has considerable financial leverage.

To this end, NBS has instituted cooperative and collaborative programs with several groups to improve the quality of materials property data. In the area of phase diagrams, three joint programs serve as the focal point for worldwide activities:

Alloys - American Society for Metals (ASM)
Ceramics - American Ceramic Society (ACerS)
Polymer Blends - Society of Plastics Engineers (SPE)

In these programs, the technical societies are responsible for seeking financial support from the user community. To date, ASM has nearly reached its goal of four million dollars and ACerS is well on its way to its goals. The NBS-SPE program has just started.

In addition, the societies are responsible for dissemination of the outputs, through publication of journals and handbooks and preparation of computerized data bases.

NBS is concerned with the technical accuracy of the data themselves. In doing this NBS draws upon technical expertise both internally and throughout the world. The computer plays an important role in the evaluation process, in calculating equilibrium and metastable extensions using thermodynamic models, and in developing graphical representations. For multidimensional systems, the computer has the ability to display two-dimensional slices as requested by the user.

Corrosion data and mechanical properties are two areas where NBS has recently begun evaluation activity. A joint program with the National Association of Corrosion Engineers (NACE) has been started to improve the quality of thermodynamic and kinetic corrosion data. Also, a number of pilot studies in the mechanical property area are beginning. Data on wear are also very important in designing products to perform in a specified manner. An additional complication is the need to specify the wear mode and to identify important parameters. Evaluation work in this area lies in the future but its importance is substantial.

All these evaluation activities reflect an increased awareness of the immense economic value of more reliable materials data.

Access/Dissemination

Providing better access to materials property data is a necessity in improving the quality of design and materials selection in U. S. industry. There have been several meetings and reports related to computerized materials data systems, with a 1982 workshop at Fairfield Glade, Tennessee, the most notable. This workshop dealt with general issues, e.g., what are the needs, opportunities, and problems associated with achieving computer access to reliable materials data. The attendees concluded not only that there were no technical barriers to building such a system, but also that it was in the best interest of the United States to move ahead quickly.

There are many advantages to a computer system versus a paper system, most notably currency, speed and accuracy of search and retrieval, and the facility for material/property matrix inversion. In addition, it is possible to interface with design algorithms and CAD/CAM systems and to build in such features as automated graphics and behavior prediction.

Perhaps the most important of these, material/property matrix inversion, is not possible with a paper system. This capability makes it possible to find all materials that have certain specified properties, a process which is carried out imperfectly, at best, now.

Building a computerized materials data system, however, does involve overcoming problems which are not as simple as those encountered with financial or business data. Among these are:

- Multiple descriptors
  - Material history
  - Processing
  - Test methods
  - Structure

- Varied format
  - Text
  - Numbers
  - Graphs

- System Development
  - Data Evaluation
  - Access
  - Standards
  - Diverse users of system
  - Questionable economics

The matter of questionable economics in creating the system refers to the difficulty in showing that better data or better access to data has a predictable effect on production costs, warranty costs, operational costs, etc. To date, only "hand-waving" arguments have been used; however, more detailed justifications are clearly needed.

The problem of standardization is also important. Presently, the few computerized materials data bases that do exist cover only a limited number of properties and/or materials. The number of data bases will grow but may do so in an uncorrelated way. The user community will demand that these data bases be linked together in some way such that all are accessible to a user via a network. For this to happen, appropriate standards need to be developed. If one simply itemizes the number of possible combinations of materials designation, property designation, and test methods and units, the resulting chaos is evident.

NBS should play a lead role in addressing these two issues, which will speed progress in making computer access to materials data a reality.

Prediction/Modeling

Regardless of the amount of work, all needed data for all possible situations will never be generated, evaluated, and made available. Consequently, a powerful positive use of computers is in directly extending data over a range of parameters not explicitly covered (interpolation) and to new ranges (extrapolation).

One example of how computers aid this process is in the phase diagrams of polymers. These have an additional complication in that the molecular weight of the polymers greatly affects the phase stablility. Using renormalization theory and the power of the computer to make the mathematical transformations, large amounts of data can be systematized. More importantly, new data can be predicted, which greatly reduces the need for costly experimental measurements.

NBS and the technical data community need to increase access to and the quality of materials property data. These efforts should emphasize:

- Evaluation - Need validation methods to assure accuracy and reliability.

- Cooperation - Both evaluation and computerization are tasks too large for one group to accomplish; NBS must help lead and actively. encourage participation of others.

- Standardization - Data bases from different sources cannot be linked without standard terminology and formats.

- Justification - Better understanding of the benefits is required to obtain the needed resources.

REPORTS OF WORKING PANELS

Nine Panels were set up to discuss the following topics in the context of selected important classes of data:

- o New needs for data arising from changing use patterns, especially those changes introduced by computers.
- o The scientific basis for data correlation and prediction.
- o Problems of compatibility and standardization of computerized data bases.
- o General prospects for computer-based data dissemination.

In addition, a tenth Panel addressed more generic aspects of standardization, compatibility, and related issues. The reports of these Panels follow.

1. Thermophysical Properties of Fluids

Chairman: Max Klein
Gas Research Institute

Secretary: John Gallagher
National Bureau of Standards

This Panel focused on the needs of design engineers and other industrial users of data on the thermodynamic and transport properties of fluids. It concluded that adequate computer hardware will soon be available to meet the needs of the design engineer. A personal computer will provide much of the needed capability and will be linked to a mainframe unit for calculations and access to data files beyond the capability of the desk-top unit. More powerful hardware will be required only for the associated scientific efforts, such as developing accurate intermolecular potentials needed for improvement of predictive models and extending the techniques to complex biochemical systems.

The rapid development of the hardware has outstripped the development of the data bases and associated software. The quality and comprehensiveness of automated data bases must be improved. A concise estimate of accuracy should be provided along with some type of condensed reference so that the data can be traced back to their source if the estimate of accuracy is of great importance. DIPPR is making a start in this direction. The limits of applicability of equations used to express the data should be indicated in all data bases.

The work on existing data bases should be better coordinated and standards should be developed to assure compatibility between data bases. This must be an international effort but with a strong U. S. presence. American industry can benefit greatly from data base activities in other countries if problems of compatibility and quality control can be solved.

Generic software programs such as nonlinear fitting techniques should be intercompared and standard data bases developed for the calibration of new industrial correlations and the development of system-modeling methods. These are natural functions for NBS.

A subtantial program is needed to develop new scientific understanding for the purpose of preparing accurate reference data. At the present time, different models or equations are being developed for different properties which are thermodynamically related. The development of integrated unifying molecular models will enable thermodynamically consistent sets of equations to be prepared. Such unifying models will become increasingly important as users couple sets of equations for different uses and integrated engineering systems design becomes more common. The models must be able to handle all fluids of industrial importance, including polar compounds with complex structures.

NBS should adopt a leadership role in coordinating the development of data bases, identifying the most important data sets, evaluating and developing interfaces among data bases, and initiating long-term unifying scientific research.

In summary, the Panel concludes that:

- o Needs for better fluid property data are pervasive in the chemical, energy, and electric power industries.
- o Hardware needs of design engineers have been largely met.
- o Automated data bases providing statements of accuracy and traceability are needed.
- o Standards for assuring compatibility between data bases are essential.
- o A long-range scientific program is needed to provide an underlying unifying molecular basis for predictive equations.

2. <u>Thermochemical Data</u>

Chairman: Malcolm W. Chase
Dow Chemical Company

Secretary: Eugene Domalski
National Bureau of Standards

The Panel believes that improved thermochemical data are needed for organic, inorganic and polymer systems, radicals and active intermediates, singly and in a variety of solutions both at low and at high temperatures. Needs are found in industrial and academic chemistry, geochemistry, and biochemistry, including living systems.

More comprehensive reference data of better quality are required. In supplying these needs, maximum use should be made of quantum mechanical and statistical mechanical techniques and knowledge of molecular structure and energetics. At present, a range of techniques is needed depending on the complexity of the systems. Theoretical and semi-empirical predictive techniques should be developed, but it should be recognized that selected evaluated data provide the starting point and the means of verification for all correlative and predictive methods.

Computers can increase the efficiency and capability of data centers in information storage and retrieval, data manipulation and dissemination, and the development of methods for correlation and prediction. NBS should play a leadership role in coordinating and developing computerized data bases and dissemination methods.

Methods of dissemination are undergoing change. At present, the publication of tables is predominant. In the near future, computerized products which generate needed values from equations will predominate. Later these will be coupled to front-end software which will assist the user in making calculations. It will be necessary for all computerized data bases to contain statements concerning accuracy, range of application, and references to more detailed documentation.

Data bases are dynamic in nature. New experimental data and theoretical techniques offer opportunities for continual improvement, and new user needs dictate frequent changes. Thermochemical data are interdisciplinary, and their compilation requires access to many sources of information. Activities in the thermochemical area should be coordinated so that access to new information can be provided to all and the recommended data bases can be readily updated.

The principal conclusions of the Panel are:

- NBS should be the focal point for the exchange of annotated bibliographies, data collections, and programs for analyzing and correlating data.

- Dissemination of thermochemical data should become computerized within a five-year period. As a first step, magnetic tapes with brief format information can be provided. Interactive front-end programs and computational routines should be made available in the next stage. Products should be provided for large, mini- and micro-computers.

- All automated data bases should contain information on uncertainties, range of applicability, and reference to a description of the evaluation process.

- NBS should play a leadership role in the dissemination of thermochemical data, working closely with professional societies, trade associations, and the commercial sector.

- A long-range program should be initiated to improve the theoretical basis for the evaluation of thermochemical data and to develop improved techniques for the correlation and estimation of data.

3. Chemical Kinetics

Chairman: John Barker
SRI, Inc.

Secretary: Alberta Ross
Notre Dame

The Panel reviewed the many applications for which data on chemical kinetics are used. In biotechnology the kinetics of enzyme reactions are of major importance. Kinetics data are needed in the study of environmental problems such as ozone depletion, acid rain, and pollution formation. Industrial applications range from petroleum cracking and the synthesis of new compounds to plasma etching, laser isotope separation, studies of combustion efficiency, and metallurgical processing. Furthermore, the field is very diverse; some users are dealing with elementary reactions while others are concerned with the rates of complex processes. As a result, there is a hierarchy of data and of access needs. These might be characterized as follows:

1. Advice of experts
2. Bibliography
3. Tabulated data
4. Evaluated data
5. Extrapolated or predicted data

Different aspects of kinetics are presently at different levels of maturity. Evaluation techniques may be empirical, semi-empirical, involve parameterized models, or be firmly based on theory. Processes in the gas phase are understood to a higher level of detail than complex condensed-phase processes. If these are to be stored together, there is need to develop a taxonomic system for storage and retrieval.

If would be desirable to have a library of computer codes for common calculations, e.g., RRKM theory, transition state theory, and the solution of systems of coupled equations.

The creation of computerized data bases in chemical kinetics is not as far advanced as in thermodynamics, partly because the theoretical basis for evaluation and prediction is not as mature. However, the time has come when the process of building computerized kinetics data bases can and should be started.

The Panel concludes that:

- NBS should take a leadership role in coordinating national and international data base development and should hold workshops to develop format and quality standards.

- Computerized data bases should be developed which are portable, user-friendly, and insofar as possible of uniform format.

- A long-term intellectual effort is needed to extend current empirical and theoretical techniques for producing reference data and to develop new ones to extend to all potential applications.

4. Spectroscopic, Crystallographic, and Other Data Used for Characterization

Chairman: R. Mooney
Standard Oil of Ohio

Secretary: R. Velapoldi
National Bureau of Standards

The Panel discussed the importance of data quality in the existing and future spectral data bases and needs for benchmark data sets and reference materials which would provide measures of quality. Critical evaluation by a group of experts in the particular area is necessary before data are included in a data base. The panel also discussed the way in which the computer already drives the entire spectral measurement system. The Panel emphasized the importance of determining the defining parameters of the data base. We need specified algorithms for data reduction and collection (standardization of techniques) so that quantitative comparisons of data bases can be made.

The Panel felt that there should be a central mechanism for interacting with users and monitoring the status of different activities. Instruments of different manufacturers now produce data in different formats; we need a common exchange format for each class of data. Data should be stored in a central location, such as NBS, for maintenance and updating. We also need faster search algorithms, as the data bases will continue to become larger and more difficult to search in a speedy fashion. Additionally, it is essential that instrumental parameters under which data were obtained are defined.

The following steps are suggested by the Panel:

- A central laboratory should provide continuity, upgrading, and updating of each data base. It is necessary that the user have some means for reporting disagreements with data in the data base, and these should be reconciled by appropriate means. Consensus bodies such as ASTM, professional societies, and manufacturers will have to be brought into the process at an early stage.

- High resolution spectral data in data bases could be degraded using specific algorithms to provide data bases with analytical (quantitative) utility under normal instrumental operating conditions. In this case, reference materials and benchmark data are critical tie points to accuracy.

- Data bases should be increasingly used as a research tool in developing innovative approaches to compound identification, trend analysis. Pattern recognition techniques will eventually allow the identification of a compound type through similarity of structural features among a set of spectra in the data base.

- Needs exist in the following areas: further characterization; near IR, far IR, and reflectance; mass spectrometry (tandem MS/MS, chemical ionization, laser ionziation); expression of NMR, UV, VIS in digital form; unification of four or five data bases in crystallography; compatibility of existing IR data bases.

5. Atomic and Molecular Data

Chairman: Bryce L. Crawford
University of Minnesota

Secretary: Jean Gallagher
University of Colorado

Atomic and molecular data describe basic properties of and interactions between photons, electrons, atoms, ions, and molecules. Its forms include energy levels, transition probabilities, line shapes, reaction rates, and cross sections. The multiple and diverse uses of these data range from the testing of fundamental theory to use as a tool for the diagnosis of plasma constituents. These data may describe excited species, highly ionized atoms, and unstable as well as stable molecules.

The Panel agreed that the principal applied uses of atomic and molecular data fall in the following areas:

1. Plasmas such as those relating to fusion, astrophysics, weapons systems, and the ionosphere.

2. Surfaces including surface processing, catalysis, and adsorption.

3. Gaseous systems such as laser systems and the atmosphere.

All users of atomic and molecular data should identify data needs and also accuracies required for their applications. Increased contact between users and the scientists who compile and evaluate the data would assist the latter group in setting priorities for its work. Special topic workshops sponsored by NBS would improve communication.

The Panel unanimously endorsed the need for computerized data bases which would allow storage and access to far greater quantities of data than can, in some cases, be published in journals. These would also enable users to identify constituents based on the measured property values.

In addition to the formal literature, the Panel cited other sources of data, including predictive models and private or special-purpose data sets. Predictive models are either general (sometimes low-accuracy) expressions to estimate the quantities of interest or scaling laws which are applied to fill gaps in sequential data. These procedures may give satisfactory estimates, but should be applied with caution and full recognition of the limitations of the method, and should not be used in place of better measured or calculated data. Local or private data sets have, in some cases, been developed as the result of an extensive program of calculations and/or to provide input to a specific modeling program. Acquisition of these data sets by the data centers to provide a centralized and comprehensive data base is an attractive idea, but there are several associated problems: These data sets would have to be identified and the cooperation of the individuals controlling them obtained. The data would have to be acquired in computer-readable form and reformatted to a standard determined for the data base. Most important, these data would have to be evaluated and, in some cases, parts or all of the data would have to be discarded because its residence in the data base would promote dissemination of meaningless data. Maintenance of the integrity of the data base is essential to retain the confidence of the scientific community.

Where possible, instead of storing data point by point, the property should be expressed analytically and the associated parameters stored. The data would then be regenerated when required by the user. Reliable optical scanners and standardization of computer hardware are needed to increase the efficiency of data collection and dissemination.

The Panel noted that it is essential for accuracy estimates to accompany data stored in data bases. Presently, much of the important and time-consuming work of evaluation is being done at the NBS Data Centers by very small groups, typically including only one or two professionals. It is impossible for so few workers to cover all pertinent cases (for example, all target species, excited states and transitions, or all energies). The most efficient approach is to divide the material systematically (for example, by isoelectric or isonuclear sequence or by group in the periodic table) and to complete the evaluation of one subdivision, using related properties of its members, before going on to the next. The results of this work can then be used in a variety of applications. The data centers are severely understaffed, however, and to obtain a comprehensive on-line data base will require an expansion of financial support to increase the number of scientists participating in the evaluation.

Aggressive leadership by both individuals and institutions is needed to coordinate worldwide efforts in the collection and exchange of atomic and molecular data, to standardize formats, to combine existing local data collections, and to stimulate communication between data centers and users. Data centers such as the Oak Ridge Fusion Data Center, emphasizing a specific use rather than a property, should be established to complement the work of existing data centers.

6. Nuclear Data

Chairman: M. Bhat
Brookhaven National Laboratory

Secretary: A. Carlson
National Bureau of Standards

Dr. Bhat described the nuclear data activities and the United States nuclear data network. He mentioned that there are presently seven or eight evaluated nuclear data files. He spoke about one of these, covering evaluated neutron reaction data, as an example. Dr. Bhat also described the "data cycle" carried out in the neutron data evaluation activities.

The nuclear data program in the United States has traditionally been much more heavily funded and better organized than programs in other disciplines. This is because it was set up to serve a top-priority activity, i.e. development of nuclear power. It was felt that the systematics of this operation could serve as an example for other disciplines.

Data needs are established through the publication of a data request list. This involves input from measurers, evaluators, funding agencies, and users. Data are then measured, evaluated, and added to the system; and data testing checks the evaluated data to complete the cycle.

This cycle has been completed five times, and work is in progress on the sixth. The result is the ENDF B file, which is the U. S. standard reference file for evaluated neutron reaction data. There is not just a single file, but a whole system. The system contains a bibliographic file on neutron data (CINDA) and another file of strictly measured data (CSISRS) which are used in data evaluations. The evaluations are run through a number of formats and physics codes, are critically reviewed and supported by documentation. Preprocessing codes are used in preparing the evaluated data to be in a form suitable for the data testing codes. The benchmark experiments used in data testing are also carried out and described in detail in the benchmark specifications. A bibliography of nuclear structure data (NSR) and the evaluation nuclear structure and decay data file (ENSDF) provide auxiliary information for the ENDF evaluation.

A Cross Section Evaluation Working Group (CSEWG) coordinates and its members carry out the evaluation work. Members from some 20 United States National Laboratories, industry, and universities take part in this large cooperative effort.

The Nuclear Data Panel wants to stress that the methodology used by the nuclear data activities is well-established and could be very profitably applied to certain other types of data.

7. Phase Diagrams of Alloys, Ceramics, and Polymers

Chairman: B. L. Rosof
Cabot Corporation

Secretary: Kirit Bhansali
National Bureau of Standards

The Panel reviewed the three major programs for phase diagram data evaluation which cover alloys, ceramics, and polymeric blends. In each of these programs, NBS is responsible for the technical quality, and the appropriate professional society is responsible for industrial fund-raising and dissemination of the evaluated information.

Phase diagrams are a graphical representation of equilibrium phases of a material at a given temperature, pressure, and composition. Historically, these have been easy to measure but difficult to calculate from first principles. However, since equilibrium is a reflection of the basic laws of thermodynamics, it is in principle possible to do the calculations if the necessary thermodynamic data are available. With the advent of computer modeling such calculations have become possible, and this has advanced our ability to correlate and extrapolate phase diagram data. The hierarchy of understanding is as follows:

- Measurement of thermodynamic data, especially for solutions and intermediate compounds

- Empirical models of the free energy of each phase

- Theoretical models of the free energy of each phase

- Expert systems for evaluation of phase data

The computer has made it possible to proceed down this list, but presently work is just beginning to reach the third stage.

While each phase diagram program has a different set of details, the same basic modeling techniques are applicable to all. The Panel believed it is very important that compatibility between the programs be maintained. This means that both the phase diagram itself and the supporting data, such as crystal structure and thermodynamics, must be the same, regardless of which program is involved.

In addition, there needs to be compatibility and standardization in the storage of data, especially in any data base system that is established. Since diagrams are needed regardless of whether a material is an alloy, ceramic, or polymer, users will want to have a common format for the different data bases to make use easier.

It is very likely that computer-based dissemination systems will eventually replace hard-copy publication of phase diagrams. The consensus was that:

- Primary use will be for evaluated phase diagrams

- Information must be easy to find and must be regularly updated

- Data bases must be searchable in a wide variety of ways

The Panel also believes that several key opportunities exist for extending the value of phase information. These include:

- o Production of higher-order phase diagrams which can be calculated, evaluated, and manipulated. Using computer graphic techniques, two-dimensional slices of these systems can be made routinely.

- o Display of metastable phases on equilibrium diagrams.

- o Extension to nonequilibrium phase formation as well as calculation of reaction paths for processing far from equilibrium (e.g., rapid solidification)

- o Introduction of nontraditional phase diagrams with other independent variables besides temperature/composition

- o Planning of key experiments to check the results of calculations and to choose between conflicting results.

8. Mechanical Properties

Chairman: Irwin Berman
Foster Wheeler Corporation

Secretary: Bruce Christ
National Bureau of Standards

It was the consensus of this Panel that the needs of design and production engineers are the primary driving force for establishing a national mechanical properties data base.

This Panel concentrated on two aspects of data activity for the mechanical properties of structural materials: evaluation considerations and computerized delivery systems. Recognizing that some efforts have already started, the Panel recommended that NBS expand its own activity and work with other groups to assure that adequate programs exist for improving the quality of mechanical property data and providing more effective access.

There is a major need for evaluation of mechanical property data. Expert opinion about the quality of data is important and, if the level of evaluation is specified for each data base, the data bases themselves are all the more valuable. However, the evaluation procedure for such data may vary according to the use to be made of the results. Manufacturing, processing, testing, and design and analysis often use the same data but in different ways. Consequently, the Panel listed three areas for attention in regard to mechanical properties:

- Evaluation of data - Must be done by materials experts who examine validity of test method, characterization of material, etc.

- Applicability of data - Differs from industry to industry, i.e., creep data needed for nuclear power applications vary from those needed for solar energy applications

- History of prior applications - Other people's experiences are important

Presently a fair amount of implicit evaluation is going on. Data sources include both government and corporate providers. However, formal arrangements need to be established. NBS has been working with professional societies to encourage them to intensify their evaluation activities. This should continue. We know the engineering community is willing to work together. For example, within ASME, over 4500 people attend six meetings a year to work on the boiler code. Once the community makes the commitment, the personnel will be there.

The work on computerized materials data systems undertaken by the Metal Properties Council (MPC) is important and should be strongly supported. Computer access to these and other data is essential today and will include benefits such as quick delivery, exhaustive searching via a wide variety of search patterns, incorporation of auxiliary information, convenience for making correlations and scientific modeling, easy graphics, and inexpensive storage of large amounts of data. A major barrier to progress in building a national mechanical properties data base is lack of a detailed study of its economic benefits. Clearly, working engineers want computer access, but top management still needs to be convinced. A careful study of the benefits is needed. The NBS studies of the costs of fracture* and corrosion** in the U. S. economy seem to be a reasonable starting point for such a study.

The other significant barrier is the initial investment in the system. One estimate is $3 million dollars a year for five years to establish a system of a size that gains user acceptance.

In addition to these nontechnical barriers, major technical work needs to be done on standardization, especially with respect to the reporting of test data and designation of materials. As regards the scientific basis for data correlation and prediction, the Panel recognized that theories of the macroscopic mechanical properties of solids are in the early stages of development, and that the proposed data base would be of value to materials scientists in establishing correlations and developing models. In fact, it is easy to imagine that mechanical properties data activity could become a working link between scientists and engineers.

In conclusion, the Panel recommends that:

- o NBS undertake studies to demonstrate the value of a computerized national materials properties data system. These should include: identifying the user community and their needs; defining the content, sources, and quality of data; and quantifying the expert and clerical labor needed to build the data files.

- o NBS, in cooperation with other groups, should undertake specific pilot evaluation projects to

  - demonstrate methodology

  - provide prototype results

  - identify needs for data standards

- o NBS should continue to work with MPC and other groups to build a computerized national mechanical properties data base. This work should include overcoming nontechnical barriers, such as start-up funding, as well as technical barriers such as standardization.

- o The user community, including both industry and professional societies, should work cooperatively in these activities.

- o The Panel felt that it is timely to initiate pilot studies <u>now</u> in support of a national mechanical properties data base.

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*NBS Special Publications 647-1 and 647-2. The Economic Effects of Fracture in the U. S. Economy, issued March 1983. Available from Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402.

**NBS Special Publications 511-1 and 511-2. The Economic Effects of Metallic Corrosion in the United States, issued May 1978. Available from Superintendent of Documents, U. S. Government Printing Office, Washington, D.C. 20402.

9. Corrosion Data

Chairman: W. W. Kirk
LaQue Center for Corrosion Technology, Inc.

Secretary: G. M. Ugiansky
National Bureau of Standards

NBS and the National Association of Corrosion Engineers (NACE) instituted recently a joint program to improve the quality of and access to corrosion-related data. This Panel considered issues associated with implementing this program and addressed the opportunities for making progress in providing needed data.

Corrosion data can be divided into two classes, thermodynamic and kinetic. Thermodynamic data deal with the long-term stability of a metal in an environment and can conveniently be represented by stability or "Pourbaix" diagrams. These diagrams show graphically whether, given a set of conditions, a material can corrode, e.g., go into solution, remain stable, or passivate.

Kinetic data are concerned with the rate of corrosion processes. Since the service life of a material is often determined by the deepest penetration anywhere, such data are vital in designing durable components.

For both types of data, a major increase in evaluation and dissemination activity will greatly aid the industrial community. To date, the NACE-NBS program has concentrated on a few pilot projects which aim at developing evaluation methodology and data formats. Eventually, the goal is to develop predictive models. All of these activities depend on computers in virtually every aspect.

The Panel made the following specific recommendations:

- Thermodynamic data
  - Implement on-line computer software to generate evaluated Pourbaix diagrams
  - Expand and improve the thermodynamic data base used in making such diagrams
  - Develop models for regions of enhanced corrosion such as at surface-liquid interfaces
- Kinetic data
  - Continue development of evaluation methodology and extend work to other types of corrosion
  - Establish suitable presentation formats for kinetic data

- Develop predictive models, especially for localized corrosion

- Set up computerized data bases

o General

- Explore the use of expert systems, operating on verified data bases, to aid the design of corrosion resistance

- Include all materials (metals, alloys, ceramics, polymers)

- Eventually, begin evaluating corrosion protection methods

For all these activities, NBS should cooperate closely with industry and groups such as NACE to ensure consistent priorities and real user involvement. The main obstacle lies not in the level of scientific understanding but in lack of adequate funding. NACE should begin fund-raising efforts, and NBS should increase their level of support. In view of the high cost of corrosion ($150 billion/year), the potential payoff is enormous.

10. Standardization, Compatibility, and Related Issues

Chairman: R. Wigington
Chemical Abstracts Service

Secretary: B. Molino
National Bureau of Standards

This Panel had the charge of dealing with the more generic aspects of standardization and compatibility and took as given many of the general questions posed to the other Panels. Thus it assumed that there are new and rapidly growing data needs in science and industry, that there is usable methodology for data validation and prediction, and that computer-based dissemination and the use of numerical data are becoming more widespread and of greater significance to the economy and will become even more so in the next few years.

To make computers more than just a passive link in human-to-human communications, and for modern information technology to be an effective tool in augmenting human intellect and productivity, the data to be communicated and operated upon, whether from files or user-generated, must be unambiguously interpretable by mechanical processes. Because the data and processes are the products of many people and organizations over extended periods of time, an appropriate standardization level is required to hold them all together. This standardization must limit by prescribed formats and coding but at the same time be adaptable to meet future needs.

Presently there is a diverse environment surrounding what is to be standardized and for what purposes. There are spectra of variations to be considered: mainframes versus personal computers, centralized versus decentralized systems, costs of communication versus storage costs, relatively stable data versus rapidly changing data. Among these diverse conditions, the approaches to standardization vary considerably.

The Panel concluded that there are definite differences in the approaches to standardization of such things as on-line handbooks, which are basic information, storage, and retrieval problems, and standardization for data-driven design and manufacturing. Also, the requirements for standardization, when dealing with a computer-to-computer environment, are much more demanding than when dealing with a human/paper system since, in the latter case, individuals can bridge most gaps in communication. At the same time, however, improving computer technology is providing more sophisticated means for transformations among equivalent representations as well as the tools to facilitate the use of the results.

Standardization is basically a means for disciplining an activity or process. Fundamentally, it is motivated by the need to take advantage of economies of sharing, not only for facilities but also labor (specifically, intellectual exercise), thus avoiding errors and duplication. In spite of these theoretical economic advantages, at present there seem to be few, if any, market-driven incentives for standards for data interchange. The Panel did not arrive at a recommendation on how to unlock this potential.

In moving towards standardization, the working Panel, in a practical approach, recommended working on restricted areas of coherent interest; for example, encouraging each discipline to develop its standard descriptive nomenclature. This has been a common practice, and successes were cited such as the DIPPR project, the crystal data projects, and the activities presently underway in alloy, ceramic, and materials property data. We should provide common influence, where practical, but we cannot expect--at least, not yet--uniformity among the various classes of data of interest.

One firm consensus of the Panel in establishing data standards is to use the descriptive level to standardize how one describes the data rather than to use highly detailed representations within the data elements themselves. It was agreed that this standardized description must also include means for describing the context and validity of the data.

Basic computer technology standards are being developed by the computer field in general, and this Panel recommends using these whenever possible. NBS is a Federal center for these activities, through both the FIPS program and the collaborative efforts with ANSI and ISO for national and international standards. Relevant standards for business and economic data should be examined, used when possible, and extended where necessary.

In addition to its leading role in the evaluation of numeric data, it is very appropriate for NBS, and OSRD in particular, to play a significant national part in the standardization that will eventually pull all numerical data efforts together. NBS should also continue to be a national focal point for international activities through such organizations as CODATA and IUPAC.

In summary, there is no secret or magic formula for achieving standardization. The only practical approach is to select cohesive communities of users and work within these groups to demonstrate the utility of adopting common methods. One can then build on this demonstrated utility and, in so doing, make definite advances in reaching conclusions for problems of solvable scope.

APPENDIX I

THE EFFECT OF COMPUTERS ON THE GENERATION AND USE OF TECHNICAL DATA

Program

Monday, March 19 — **David R. Lide, Jr., Presiding**

9:00 a.m. Opening Remarks - Clarence T. Brown, Deputy Secretary of Commerce

9:15 a.m. The Federal Role in Stimulating Industrial Competitiveness - John McTague, Deputy Director, Office of Science and Technology Policy

10:00 a.m. Coffee Break

10:30 a.m. Computerization of the Design/Production Cycle - Michael Wozny, Director, Rensselaer Polytechnic Institute, Center for Interactive Computer Graphics

11:15 a.m. Materials Data for the Factory of the Future - Michael T. Jefferies, R & D Manager, Engineering Physics Laboratories, General Electric Company

12:00 Noon Challenges for the Technical Data Community - Ernest Ambler, Director, National Bureau of Standards

12:45 p.m. Lunch

1:30 p.m. Fluid Properties and Thermochemical Data

David W. H. Roth, Jr., Director, Office of Science and Technology, Allied Corporation

Neil Olien, Chief, Chemical Engineering Science Division, National Bureau of Standards

2:30 p.m. Atomic, Molecular, and Nuclear Data

James J. Wynne, Watson Research Center, IBM

Wolfgang Wiese, Chief, Atomic and Plasma Radiation Division, National Bureau of Standards

3:30 p.m. Coffee Break

4:00 p.m. Materials Performance Data

Jack H. Westbrook, Materials Information Services, General Electric company

Louis R. Testardi, Chief, Metallurgy Division National Bureau of Standards

Tuesday, March 20 — **Donald R. Johnson, Presiding**

9:00 a.m. Charge to the Working Panels - David R. Lide, Jr., Director, Standard Reference Data, National Bureau of Standards

9:15 a.m. Working Panels will meet in rooms to be assigned

12:45 p.m. Lunch

1:30 p.m. Working Panel reports and discussion

4:00 p.m. Conclusion of Workshop

LIST OF WORKING PANELS

Panel	Chairman	Scribe
1. Thermophysical properties of fluids	M. Klein Gas Research Inst.	J. Gallagher NBS
2. Thermochemical data	M. W. Chase Dow Chemical	E. Domalski NBS
3. Chemical kinetics	J. Barker SRI International	A. B. Ross Notre Dame
4. Spectroscopic, crystallographic and other data used for characterization	R. Mooney Standard Oil of Ohio	R. Velapoldi NBS
5. Atomic and molecular data	B. Crawford University of Minnesota	J. Gallagher University of Colorado
6. Nuclear data	M. Bhat Brookhaven National Laboratory	A. Carlson NBS
7. Phase diagrams (alloys, ceramics, polymers)	B. Rosof Cabot Corporation	K. Bhansali NBS
8. Mechanical properties	I. Berman Foster Wheeler Corporation	B. Christ NBS
9. Corrosion data	W. W. Kirk LaQue Center for Corrosion Tech., Inc.	G. Ugiansky NBS
10. Standardization, compatibility, and related issues	R. Wigington Chemical Abstracts Service	B. Molino NBS

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APPENDIX III

STUDIES AND ARTICLES DEALING WITH NEEDS FOR RELIABLE PHYSICAL, CHEMICAL, AND MECHANICAL PROPERTY DATA

A SELECTIVE BIBLIOGRAPHY
MARCH 1984

Towards a National S&T Data Policy: A Workshop - coordinated by Committee on Science and Technology, U.S. House of Representatives; Congressional Research Service, Library of Congress; Numerical Data Advisory Board, National Academy of Sciences, 1983.

This workshop approached the question of establishment of a national scientific and technical data policy through a number of talks and discussions which examined data requirements in industry, agriculture, and other sectors. Many specific examples were given of the benefits of reliable, widely available data bases.

Gilbert Gude, Director, Congressional Research Service, said in his concluding remarks:

"Scientific and technical information will be vital to the growth of high-technology industries in the future as well as to the revitalization of today's manufacturing and agricultural sectors. Effective management of these information resources has the potential to boost productivity and increase the competitiveness of American business. The ability of policy makers to respond to changes brought by scientific and technical information and to provide guidance for the utilization of these resources will have a direct impact on the economic and social condition of the Nation in the future."

National Needs for Critically Evaluated Physical and Chemical Data - Committee on Data Needs, Numerical Data Advisory Board, National Research Council, 1978 (Walter H. Stockmayer, Chairman).

This is the report of a study on data needs, current U. S. efforts to produce evaluated data, and the benefits to be expected from a comprehensive evaluation program. The major recommendations were:

"1. The present annual support for organized data evaluation activities of slightly under $7 million should be increased over a period of five years to $18 million. For reasons outlined in Chapter 8 this support will have to come primarily from the Federal Government.

2. When a particular mission relies heavily on results from a field of research, responsibility for data compilation and evaluation in that field should be accepted by the agency responsible for the mission. The Office of Standard Reference Data of the National Bureau of Standards should be responsible for categories of data of very broad utility and for general coordination of the overall system.

3. Each agency should be required to place its responsibility for data compilation and evaluation on one key official at a level high enough to ensure that the agency's responsibilities in this area will be fulfilled."

The Department of Energy: Some Aspects of Basic Research in the Chemical Sciences - Committee on Chemical Sciences, National Research Council, 1979 (Robert E. Connick and Bryce Crawford, Jr., Cochairmen).

This NRC report assisted the Department of Energy in defining its needs through a look at basic chemical research in selected fields, as well as certain research policy issues.

Under research policy issues, a section on Critically Evaluated Data contained the following:

"The Directors of the Divisions of Materials Sciences and Chemical Sciences of OER have both expressed to this Committee their concerns about the inadequacy of reliable evaluated data. Data needs related to DOE programs range over chemical sciences in the broadest sense, from spectroscopy to combustion engineering, from solid-state properties to corrosion. Chemical data pertinent to DOE programs include spectroscopic constants (from X-ray to nmr) for atoms, ions, and gaseous molecules; fundamental kinetic and transport data, such as rate constants, diffusivities and conductivities; thermodynamic data (including data for surfaces and data at extreme conditions); crystal structures and phase diagrams; electrochemical data; state properties of solids, liquids, gases, and plasmas.

Data evaluation requires a considerable investment of time and money in the initial installation of literature-retrieval and data-processing techniques; data evaluation also requires highly trained people. For these reasons, it is important to ensure the continuity of groups with experience in critical evaluation and tabulation. The recommended program of continuing evaluation will have long-term applications for a wide range of fields, and it is essential to maintain a level of activity that will keep pace with the flow of new data in the literature."

Improving R&D Productivity: The Federal Role - Lewis M. Branscomb, Science, 14 October 1983.

This article focuses on the importance of evaluated data to R&D productivity, and the Federal role in assuring the availability of such data. The article summarized:

"Despite widespread concern about lagging productivity growth rates and renewed interest in research, federal support for the review and packaging of hard-won new knowledge continues to languish. Yet accurate, accessible data are critical, not only in every R&D project but also in the most advanced manufacturing processes. Ensuring reliable, retrievable data is not a function that can be left to the professional societies, the publishing industry, or the private sector. In this article a six-point national science and technology data policy is proposed, and it is suggested that progress ultimately will depend on an overall science and technology policy, the first priority of which is to make available existing knowledge."

Materials Properties Data Management - Approaches to a Critical National Need - National Materials Advisory Board. National Research Council, 1983 (William F. Brown, Jr., Chairman).

This report results from a study of the needs for storage, dissemination, and analysis of materials properties data vital to the design process. One conclusion of this report states:

"The federal government and the private sector should work cooperatively to establish a national computerized materials properties data bank network that would efficiently provide carefully evaluated information to our industrial designers. Active participation of the federal government is initially required because start-up costs cannot be rapidly recovered and because the whole nation will benefit from the existence of such a network."

Computerized Materials Data System: The Proceedings of a Workshop Devoted to Discussion of Problems Confronting Their Development - J. H. Westbrook and J. R. Rumble, Jr., Editors (1982).

These are the proceedings of a workshop which brought together a number of international experts to discuss the problems associated with the establishment of computerized materials data systems.

As part of the discussion of barriers to such systems the proceedings state:

"Two other important political factors also should be considered. First, a new institutional framework on both the national and international levels is needed to coordinate and manage databases. On the national level an organization that enables all the groups listed above to cooperate has become both necessary and urgent. Internationally the need is greater because of language and nomenclature problems and the previously mentioned obstacles to data flow across national boundaries. Second, the timing of the creation of a comprehensive database system through the gateway concept is critical. It is a distinct possibility that a system of databases developed elsewhere--for example, Japan--will offer such compelling and efficient services that the rest of the users in the world will turn to it because of necessity and cost/ benefit advantages. Also, a Tower of Babel effect could soon come about for lack of a coordinated development of mutually compatible files, languages, and database management systems. That is, over a short period of time so many independent databases could develop that bringing them together later in some kind of effective, rational functioning unit might become well-nigh impossible."

Mechanical Properties Data for Metals and Alloys: Status of Data Reporting, Collecting, Appraising, and Disseminating - Panel on Mechanical Properties Data for Metals and Alloys, National Research Council, 1980 (James A. Graham, Chairman).

This report assesses the status of mechanical property data compilation and evaluation and recommends a cooperative national program to provide the data needed by industry and Government.

The panel recommended that:

"There is a continuing need for the organizations concerned with mechanical properties cooperatively

(a) To develop and improve the uniformity of test methods and data reporting;
(b) To develop definitions of nomenclature and properties;
(c) To develop property data appraisal procedures;
(d) To disseminate data including those evaluated in the process of developing test methods;
(e) To provide lists and disseminate information on test methods, data reporting, measurement standards, definitions, nomenclature, and appraisal procedures;
(f) To coordinate data efforts and assess data needs through organizing active committees, symposia, conferences, workshops, and other methods."

<u>Thermophysical Properties for Synthetic Fuels</u> - (A report prepared by the Working Group on Thermophysical Properties of Synthetic and Related Fuels for the DOE, J. Kestin), Chairman, 1982.

This report surveys the need for a data base of physico-chemical properties of substances required by the emerging synfuels industry.

In the conclusion, steps leading to the creation of a reasonable data base are listed.

"The steps which it is necessary to take consist of

- the development of methods to sample and to characterize samples from process streams

- the development of improved predictive correlation methods to cope with the increased complexity

- the creation of a base of carefully performed measurements on pure components and on prepared mixtures for the validation of correlations

- the expansion of existing experimental facilities in the country in support of the program of measurements

- the creation of a mechanism or center for the coordination of activities and to secure a continuous exchange of ideas and methods between industry and academic and government laboratories and between experimentalists, theoreticians and correlators."

Transactions of the Conference on Thermodynamics Research Requirements on Fossil Fuel Processes - Science Applications, Inc., 1979.

The objective of the conference was to consider classes of thermodynamic research essential to the development of a program for the Fossil Fuel Extraction Division of DOE. Strong emphasis was placed on thermodynamic data requirements.

The following statement was part of the overview of the section on Thermodynamic Properties:

"In the following section, topics of the highest priority are described to provide design engineers with data for sound process design. It is recognized that equations-of-state ranging from cubic equations of the van der Waals type to corresponding states and group contribution descriptions would be an effective way of using a minimum of laboratory data to describe a wide variety of relevant process thermodynamic properties. Implicit in such equation of state development is the need for fundamental data in areas such as molecular dynamics. Also experimental measurements to support parameter determination for equations of state are needed.

Equations of state must be developed to handle multicomponent, multiphase predictions. It would be desirable if these predictions can be made using experimental measurements on binary systems."

Value of the Energy Data Base - King Research, Inc., 1982.

This report documents an assessment of the Energy Data Base (EDB) of DOE's Technical Information Center. The EDB provides access to a broad range of information in the world's energy literature, of which numerical data forms one component. The study attempted to quantify the benefits of making this information readily available to the energy R&D community. One paragraph in the Executive Summary states that:

"The latter figure, $3 billion savings in labor and equipment from the EDB products and services, can be roughly translated into productivity. If it is assumed that, with the EDB, research and development costs $5.8 billion for a given level of output, without the EDB the same output would require an investment of $8.8 billion. This is an increase in productivity of about 52 percent. This says that to accomplish the same R&D output without TIC information services, the R&D budget would have had to have been $3 billion higher."

Development and Use of Numerical and Factual Data Bases - AGARD* Lecture Series No. 130, North Atlantic Treaty Organization, Oct. 1983.

(*Advisory Group for Aerospace Research and Development)

An international group of speakers presented a two-day program of talks on reliability, availability, accessibility, utilization, and management of numerical data bases. The written versions of these talks are contained in this volume.

The Preface states:

"Numerical and factual data, as sources of information for all levels of aerospace and defense R&D management and staff activity, are becoming increasingly important. These data are necessary to support research and engineering efforts in all fields. They are also becoming increasingly important to support or assist in the decision-making process. Today, a number of numerical data bases are available through national information centres and others are available from academic or commercial information sources. Data in many of these data bases can be retrieved and manipulated in display systems currently available. There is, however, a great need to improve the quality, reliability, availability, accessibility, dissemination, utilization and management of these data."

<u>Workshop on Data Quality Indicators: Summary Report and Recommendations</u> - sponsored by Chemical Manufacturers Association, 1982 (Carlos M. Bowman, Chairman).

This workshop addressed the need for more reliable data and better methods for indicating the level of reliability. The emphasis was on data relevant to environmental quality and health effects. From the Executive Summary:

"The proliferation of computerized data bases has increased the amount of data and information available. Unfortunately, many of these data bases do not provide the user with any indication of the quality of the data retrievable from the system. Tracing the origins of a particular value is often difficult, if not impossible. Association of appropriate quality indicators with the information in these data bases could provide a user with sufficient information to judge the applicability of a particular datum value for a specific use."

<u>Current Trends in Atomic Spectroscopy</u> - James J. Wynne, Physics Today, November, 1983.

Current activities and trends in atomic spectroscopy are discussed in the context of new experimental tools such as synchroton radiation and lasers, and the needs for evaluated spectroscopic data are outlined for a variety of applications. In a major section on Compilations and Tabulations, the author states that:

"Data banks containing the best values of the measurable quantities of a field are an indispensable addition to the primary literature. In atomic spectroscopy, these data banks include refined and evaluated information on quantities such as line positions, line strengths and energy levels. The entries either come from laboratory measurements or from various theoretical or empirical calculations. Evaluated data are important to the scientific community for a number of reasons, including the following:

- The process of compilation often reveals fundamental inconsistencies or conflicts in the data

- Applied spectroscopists require a rapid means for obtaining reference data
- The compilations are a pathway to the primary literature, which presents the experimental and computation work
- Theorists depend on reliable data with which to develop models and compare their predictions
- The compilations indicate the state of our knowledge.

Report of the Subcommittee on Energy-Related Atomic and Molecular Science - Committee on Atomic and Molecular Science, National Research Council, 1976 (Benjamin Bederson, Chairman).

This report documents the significance of atomic and molecular science to energy-oriented research, development, and technology.

In the Appendix on "Scientific Data: Evaluation and Dissemination," the subcommittee concludes:

"One of the more complicated aspects of the application of atomic physics or chemistry to research in the field of energy is the diversity and the magnitude of the various programs. A partial listing of the energy research programs in which atomic or molecular data are needed would include all the areas discussed in this report. Established data centers are in a position to supply most of the atomic needs of these various programs. The chief need for an additional data center is probably for molecular data; a 'Data Center Steering Committee' could provide a valuable focus for establishing national data accumulation and evaluation policies in atomic and molecular science and for serving as a clearinghouse for channeling data requests by users."

Current Trends in Atomic Spectroscopy - A report prepared by the Committee on Line Spectra of the Elements - Atomic Spectroscopy, National Research Council, 1984 (James J. Wynne, Chairman).

This report includes a review of existing atomic spectral data bases and summarizes gaps in our knowledge of atomic parameters. In regard to computerized data bases, the report states:

"A major problem associated with modern data compilations is that of making the information readily accessible. Recourse to highly automated procedures is inevitable and essential for speed as well as convenience...the necessary hardware is readily available and there are no technological roadblocks for immediate implementation."

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The National Bureau of Standards held a Workshop on the Effect of Computers on the Generation and Use of Technical Data on March 19-20, 1984. The Workshop addressed changes in the generation, dissemination, and use patterns of scientific and technical data which are occurring as a result of the widespread introduction of computers. The principal conclusions of the Workshop are summarized in this report. Synopses of the talks presented at the Workshop and reports of the working panels which met to discuss specific topics are also included.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

CAD/CAM; chemical data; computers; computer graphics; data bases; engineering data; physical data; on-line systems

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