Computerization and Networking of

Materials Data Bases

Glazman/Rumble
editors

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Foreword

The 1st International Symposium on Computerization and Networking of Materials Property Data Bases was held 2–4 Nov. 1987 at Philadelphia, PA. The symposium was sponsored by ASTM Committee E-49 on Computerization of Material Property Data. John R. Rumble, Jr., National Institute of Standards and Technology, and Jerry S. Glazman, Combustion Engineering, served as chairmen of the symposium. John R. Rumble, Jr. and Jerry S. Glazman are editors of the resulting publication.

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Overview

Using computers to deliver materials information is now a reality. Many groups that previously published are now using data bases to make available to the general public property data for metals, alloys, composites, polymers, and plastics. Many more data bases are being developed for individual companies.

In spite of all this activity, building, distributing, and using materials data bases is not yet routine or necessarily easy. Of all the materials data bases that now exist, no two of them are compatible in any significant way. The user interfaces are different, the nomenclature varies, and different data are collected, even for the same test methods. Unfortunately, all this incompatibility lies on top of the chaotic hardware and software situation.

ASTM has established Committee E49 on Computerization of Material Property Data to develop standards and guidelines for materials data bases. The goal is not to impose rigidity or hinder innovation, but rather to develop a common basis for handling materials data on computers. The key questions being addressed are as follows:

1. How can materials be described and identified in data bases?
2. What data items must be reported with test results to make them meaningful?
3. How should these data be reported? In what format?
4. What information should the user interface contain?
5. How can the developed guidelines be used in data base building?
6. How can data from two different data bases be accessed and combined?
7. How do you indicate the quality of data in data bases?

The standards will allow builders of materials data bases to draw on the experience of the community in answering these and similar questions. Users will be able to access different data bases more uniformly. Distributors of data bases will be able to maintain compatibility from one data base to another.

Enough progress has been made in the two years the Committee E49 has operated to make it worthwhile to involve the materials data base community in an open forum to exchange ideas on what has been done and what needs to be done next. That forum became the First International Symposium on Computerization and Networking of Materials Property Data Bases, held in Philadelphia, PA, on 2–4 Nov. 1987, and attended by 128 experts from 11 countries. The presentations covered many aspects of materials data bases:

- Standards activities
- National and international activities
- Emerging issues
- Impact
- Data base projects
- Cooperative data base programs

The papers in this volume are grouped according to these categories. Before describing them, some general conclusions can be drawn.

The state of the art of materials data bases had advanced rapidly with respect to the coverage of materials. Of the major classes of structural engineering materials, polymers, metals, and composites all have substantial data bases. These are being distributed both publicly and within private organizations. The general situation seems to be the same in the United States, the European Community, Japan, and China.

Aside from the coverage, the situation for materials data bases can best be described as lots of ideas and many goals but few successes. Some important points can be made:

- Standards for materials data bases have considerable support, and there is a strong desire for international compatibility of these standards. The standards, however, are not yet in place.
- Most industrial countries have made a commitment to develop an integrated network of individual data bases. Implementation varies considerably and most efforts have found that the work is going more slowly and costs more than originally anticipated.
- The impact of materials data bases is recognized to be indirect, thus making its calculation very difficult. This is further reflected by the difficulty some data base providers have had in getting started.
- Personal computer data bases of materials data are much further advanced than networks. Although individual PC data bases have attractive manipulation and display features, they do not now contain very much data.
- Very few data bases have a full range of test data and most do not include property data as a function of temperature or other conditions.
- Expert systems linked to user interfaces and integration of materials data bases into other computerized engineering tools are high-priority goals, but more research must be done.
- Significant problems still exist with respect to capturing the richness and complexity of materials data.
- In the United States, cooperative data base programs have been very successful in drawing upon industrial and government resources to improve the quality and accessibility of materials data.

Standards for Materials Data Bases

In his paper, Kaufman describes the activities of ASTM Committee E49 on Computerization of Materials Property Data. A full discussion is given of the types of standards being developed. Westbrook gives a detailed example of one E49 standards area, the identification of metals and alloys. Reynard discusses international aspects of materials data base standards, focusing on the recent activities of the Versailles Project on Advanced Materials and Standards (VAMAS). Great concern has been expressed by many people in this field that standards developed by individual countries must be compatible, and VAMAS, in conjunction with E49, has been defining the issues involved.

National and International Materials Data Base Activities

Almost every industrialized country has a major effort to make materials data bases available by on-line computer networks. The papers in this section give an overview of notable examples of these efforts. Kaufman discusses the National Materials Property Data Network, Inc., a cooperative effort between industry and technical societies in the United States to build such a network. Kröckel and Steven present the efforts of the EEC on a similar network that involves data bases from many European countries. While the goals of the two groups are about the same, the approaches are quite different as are the sources of support.

Three papers describe aspects of other national efforts for materials data bases. Lu and Fan cover activities in China, which include an impressive list of areas where work has started. Nishijima, Momma, and Kanao discuss work in Japan, especially at the National Research

Institute of Metals. Finally, Bathias and Marx give the results of a recent survey done in France on the need and acceptance of materials data bases.

The paper by Barrett covers the activities of the Committee on Data for Science and Technology (known as CODATA) of the International Council of Scientific Unions. CODATA provides a forum for cooperative data work on an international scale, and its task group on materials data bases will be important in future years.

Emerging Issues

Materials data are rich and complicated. The data themselves are an integral part of engineering and manufacturing. The interpretation of these data, especially in the context of various applications, comes close to being an art.

The set of papers in this section deals with these issues from the perspective of computerization: How to capture the complexity? How to integrate materials data bases with other software? How to incorporate expert systems?

Most of the ideas presented here are new and have not been incorporated in working systems. Some are drawn from other fields. Some are embryonic. They are important ideas and, even though some of the papers require serious reading and rereading, this will be well worthwhile. Su and Furlani have been leaders in the integration of engineering data bases, especially in computer-aided design (CAD) and computer-aided manufacturing (CAM). It is the dream of many to link materials data bases into CAD/CAM systems, and these papers give important background.

McCarthy and Grattidge have played key roles in the development of prototype Materials Information for Science and Technology system in the United States and discuss important aspects of handling materials metadata and data capture. Many of the issues raised are still problems that must be solved before large-scale materials data networks will exist.

In his paper, Iwata presents some thought-provoking ideas on the need for expert systems as part of the interface to materials data bases. The final paper of this section is by Pilgrim et al. covers an important approach to querying materials data bases.

Impact of Material Data Bases

Little has been written as to the impact that materials data bases will have on engineers in their work, or the related issue, the lack of perceived impact. Burte and Harmsworth describe how data bases affect the unified life cycle engineering concepts being developed by the U.S. Air Force. Little and Coyle cover how materials data bases relate to other work in the aerospace industry.

The other two papers look at the impact issue from the point of view of overcoming the lack of perceived impact. Martini-Vvedensky discusses the problems of starting a business based on materials data bases, while Rumble looks at various socio-economic issues that provide barriers to progress.

Materials Data Base Projects

This section of papers contains descriptions of a variety of materials data bases, built for many reasons. Petrisko, Moniz, Ranger, and Lees et al. all describe materials data bases built for their companies. Li and Ho and Newton and Gall discuss data bases built for the U.S. government. Schenck and Dennis, and Ondik and Messina cover work of the American Ceramics Society and NBS on phase diagram data bases.

Cooperative Materials Data Base Programs

Over the last decade, several large data programs in the United States have addressed industrial needs for high-quality, easily accessible materials data. These have been cooperative programs between technical societies, industry, and government.

Anderson and Laverty discuss the corrosion data program of the National Association of Corrosion Engineers (NACE) and the National Bureau of Standards (NBS). Scott et al. describe the Alloy Phase Diagram Program of ASM International and NBS, which has had many contributions from other countries. Jones and Vanderveldt cover the welding data program of the American Welding Institute. To end this section, Jahanmir, Hsu and Munro discuss the new tribology data program involving NIST, the Department of Energy, the American Society of Mechanical Engineers, and American Society of Lubrication Engineers.

Summary

The editors hope that the readers of this volume will come away with an understanding of the present-day status of materials data bases, both in the United States and internationally. There are many ideas, old and new, that should be useful. In future years, we look forward to seeing these ideas become reality.

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Standards for Materials Data Bases

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Standards for Computerized Material Property Data—ASTM Committee E-49

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ABSTRACT: ASTM Committee E-49 on the Computerization of Materials Property Data was instituted in 1986 to provide guidance to individuals and organizations building machine-readable data bases and to aid in the development of compatible and consistent sources capable of a reasonable exchange of information. In the relatively short interval since then, progress has been made in several areas, most notably in the development of formats for the characterization of materials and reporting of test data. Progress has been most rapid in the more mature and stable material classes like metals and polymers. The relative newness and lack of stability of terminology and test procedures for advanced materials will require more time and effort before major strides are apparent. ASTM Committee E-49 is also taking on the significant challenges of data exchange formats and guidelines for the evaluation of data.

Continued rapid progress in all of these areas is essential if we are to maximize the opportunity to improve the quality of materials related decisions through the use of easily accessible and exchangeable numeric performance data.

KEY WORDS: standards, materials, data base, ASTM, computer

ASTM Committee E-49 on the Computerization of Materials Property Data was formed in 1986 [*1,2*] in response to an increased recognition of the great resource value of well-documented materials property data and of their importance in high-quality decision making in materials selection and design [*3–5*]. It was one of two major developments in recent years in response to the critical need for easier direct access to more reliable numeric performance data, the other being the formation of the National Materials Property Data Network, Inc. [*6,7*]. The latter, known now as the MPD Network or sometimes simply as MPD, is a not-for-profit corporation providing U.S. engineers and scientists with easy on-line access to high-quality, machine-readable, numeric data. It was established to fill the critical need for materials selection and design decisions based upon more accurate and reliable performance information. This need was identified in several expert studies, including one by the National Materials Advisory Board [*8–11*].

The second development was the formation of ASTM Committee E 49, to develop standard classifications, guides, practices, and terminology for building and accessing materials property data bases. This committee is working with other ASTM technical committees and organizations that develop standards related to materials and their properties to bring some consensus to this explosive areas of activity. Committee E-49 will establish guidelines to aid those individuals and organizations building data bases or intelligent knowledge systems to ensure that high lev-

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els of quality and reliability are maintained and that compatibility with other sources is assured. The latter is essential if we are to be able to readily and cost-effectively share and compare data across organization lines.

The motivation for a cohesive national resource optimizing our ability to share data is particularly compelling now. Many of our traditional sources of data, such as materials producers and government laboratories, have either cut back their activities in this area or eliminated them completely. In some cases the organizations themselves no longer exist. Pressures to restructure and cut costs in the traditional materials, engineering, and heavy industry segments plus the pressure on reducing the national deficits will keep the United States in this situation for some time. Yet to meet foreign competition, we must maintain our materials know-how at a high level. The development of easily accessible electronic sources of materials property data is one significant way to do so.

The second compelling reason for a major effort in this important area is the proliferation of new, high-performance structural materials, notably composites of metals, polymers, or ceramics, or both, composing the group commonly referred to as "advanced materials." The large numbers of basic materials, plus the seemingly endless combinations of procedures by which they are assembled, make assimilation and comparison of data for these new products difficult if not impossible. Yet to shorten the time needed to commercialize these new products and establish competitive production positions, it is essential to develop guidelines and standards for handling data for these materials in high-quality, numeric, machine-readable data bases.

Finally, the effort to standardize procedures for dealing with numeric materials property data in machine-readable form is vital. This is because the development of systems for organizing and storing numeric data for retrieval greatly increases the value of our materials research dollars. In computerized systems, the individual test results are kept "alive" and accessible in well-documented form for ready comparison with newly developing materials research. A mechanism will also exist to resurrect and archive "lost" data for earlier programs, the results of which are often resident in untraceable company or laboratory files or in the drawers of the original researchers, never to be looked upon again. A concerted effort to incorporate the results of the more valuable research programs in searchable electronic sources can substantially reduce the new testing required to establish performance comparisons for competitive materials for new applications.

Background of ASTM Committee E-49

Several other groups, including American National Standards Organization (ANSI), International Standards Organization (ISO), and Institute of Electrical and Electronics Engineers (IEEE), as well as ASTM Committee E-31 on Computerized Systems [*12*] have had a significant role in establishing standards for computerized information systems. But ASTM Committee E-49 is the only one to specifically focus on the problems that arise in dealing with numeric/factual materials property data. It is worth noting the breadth of activity of these other groups, however, as indicated by Table 1 [*12*].

Committee E-49 held its formation meeting in March, 1986, primarily as a result of the concerted efforts of the National Materials Property Data Network and the National Bureau of Standards to move toward consensus (rather than arbitrary) standards for developing and accessing/transferring data. The scope of Committee E-49 is as follows:

> The promotion of knowledge and development of standard classifications, guides, practices, and terminology for building and accessing computerized material property data bases.
>
> This committee will work in concert with ASTM technical committees and other organizations that develop standards related to materials and their properties.

TABLE 1—*Standards for computerized systems and network development and operation* [12].

These standards for network development are recommended for adoption and use:

Terminology
- ANSI X3/TR-1—Dictionary for Information Systems
- ASTM E 1013—Terminology Relating to Computerized Systems

Overview
- ASTM E 622—Generic Guide for Computerized Systems

Project Definition
- Draft E3103-5—Guide for Project Definition for Computerized Systems

Functional Requirements
- ASTM E 623—Guide for Developing Functional Requirements for Computerized Systems

Functional Design
- ASTM E 730—Guide for Developing Functional Designs for Computerized Systems
- ISO 7498—Basic Reference Model for Open Systems Interconnection

Implementation Design
- ASTM E 624—Guide for Developing Implementation Designs for Computerized Systems
- ASTM E 625—Guide for Training Users of Computerized Systems

System Assembly, Installation, and Testing
- ASTM 3 731—Guide for Procurement of Commercially Available Computerized Systems
- IEEE 730—Standard for Software Quality Assurance Plans
- IEEE 828—Standard for Software Configuration Management Plans
- IEEE 829—Standard for Software Test Documentation
- IEEE 830—Guide to Software Requirements Specifications
- IEEE Draft P983—Guide for Software Quality Assurance
- IEEE Draft P1012—Standard for Software Verification Plans
- IEEE Draft P1042—Guide for Software Configuration Management
- IEEE Draft P1059—Guide for Software Verification and Validation
- EIA, ANSC X3, UL, NFPA Standards as required

System Evaluation
- ASTM E 626—Guide for Evaluating Computerized Systems

System Documentation
- ASTM E 627—Guide for Documenting Computerized Systems
- ASTM E 919—Specification for Software Documentation for a Computerized System
- ANSI X3.88—Computer Program Abstracts

These standards for network operation are recommended for study and imitation:
- ANSI X9.2—Interchange Message Specification for Debit and Credit Card Message Exchange among Financial Institutions
- IATA—Standards for data messages

The second paragraph of this scope statement emphasizes that the activities of the group do not infringe on those of other committees and organizations with expertise on materials, test methods, properties, and applications. Rather, E-49 will cooperate closely with those groups, providing the uniformity and standardization required to ensure the generation of cohesive and compatible computerized sources, and an outlet for the communication of those standards to the technical community.

Examples of current cooperative efforts with other organizations include the effort to address the characterization and presentation of data for ceramics with the American Ceramic Society. Guidelines for dealing with data for welded joints are also being established through collaboration with the American Welding Society and American Welding Institute. These functions are accomplished by the active participation of representatives of those organizations on Committee E-49. The role of the committee in such instances will be to influence the standards development work of these other groups, endorse their efforts, and incorporate them into the appropriate ASTM standards.

The activities of ASTM Committee E-49 also have the strong support and participation of the

National Bureau of Standards, notably the Standard Reference Data Program and the Institute of Material Science and Engineering, as well as of other government laboratories as well, including Lawrence Berkeley and Sandia Laboratories.

Close association and cooperation with international groups is being sought. Strong links have already been established with the Commission of the Economic Community data base network program [*13*]; the European Aluminum Association; VAMAS [*14*]; and CODATA [*15*], the Committee on Data for Science and Technology of the International Council of Scientific Unions (ICSU). ASTM Committee E 49 is filling a key role defined in the recent VAMAS report [*14*], in which the need for strong leadership in the field was cited. A cooperative position with ISO is also being sought, a goal that has been hampered by some recent personnel changes in that organization.

Four Subcommittees of E-49 have been established (Table 2). High priorities have been put on the development of data recording and computer storage formats, and therefore on the options for presenting the data. Preliminary guidelines for the working subcommittees and task groups have been written and distributed. Several individual task group activities are already underway to address specific material descriptors and test data reports. Each of the subcommittee activities will be discussed in turn below.

Standards for Material Characterization and Test Reporting

Materials Descriptors

Preliminary guidelines developed by Committee E 49 suggest that the following categories of information will probably be required to characterize all materials for computerized data systems:

- material class (metal, polymer, composite, ceramic, etc.),
- specific material within class (stainless steel, SiN, etc.),
- material designation (industry standard or experimental),
- material condition (industry standard or broad class),
- material specification (ASTM or another or both),
- material producer or source of material,
- producer lot number or number assigned by source or data base builder or both lot and assigned number,
- product form (casting, forging, laminate, compact, and so forth)
- material composition (individual lot for which data is shown), and
- fabrication history (major elements of fabrication procedure, especially those most likely to have a specific impact on material properties or performance).

TABLE 2—*E 49 subcommittees.*

E49.01—identification of materials: identifying and selecting those descriptors and coding systems necessary to adequately describe and differentiate materials for a computerized materials data base.

E49.02—reporting of material property data: development of guidelines for presentation of material properties data to be included in computerized materials properties data bases.

E49.03—terminology: oversight of the development of a standard terminology for use in building and accessing a computerized materials property data base, including definitions, nomenclature, abbreviations, and units.

E49.04—data base interfaces and functionalities: researching and developing guidelines for the transfer, processing, and presentation of materials data among distributed data bases and users, including areas such as data exchange formats, data security, search and presentation capabilities, and data quality and reliability.