Computerization and Networking of

Materials Databases

Fourth Volume

Charles P. Sturrock and
Edwin F. Begley, editors

ASTM

STP 1257

STP 1257

Computerization and Networking of Materials Databases: Fourth Volume

Charles P. Sturrock and Edwin F. Begley, editors

ASTM Publication Code Number (PCN)
04-012570-63

ASTM
1916 Race Street
Philadelphia, PA 19103
Printed in the U.S.A.

ISBN: 0-8031-2026-5
ASTM Publication Code Number (PCN): 04-012570-63
ISSN: 1050-8112

Photocopy Rights

Peer Review Policy

Each paper published in this volume was evaluated by three peer reviewers. The authors addressed all of the reviewers' comments to the satisfaction of both the technical editor(s) and the ASTM Committee on Publications.

The quality of the papers in this publication reflects not only the obvious efforts of the authors and the technical editor(s), but also the work of these peer reviewers. The ASTM Committee on Publications acknowledges with appreciation their dedication and contribution to time and effort on behalf of ASTM.

Printed in Ann Arbor, MI
October 1995

Foreword

The papers in this publication, *Computerization and Networking of Materials Databases: Fourth Volume,* were presented at the Fourth International Symposium on the Computerization and Use of Materials Property Data held in Gaithersburg, Maryland, 6–8 October 1993. The symposium was sponsored by ASTM Committee E49 on Computerization of Materials and Chemical Property Data and The National Institute of Standards and Technology. Charles P. Sturrock and Edwin F. Begley, The National Institute of Standards and Technology, presided as symposium chairmen and are editors of this publication.

Contents

Overview

The Materials Data Marketplace

Materials data are a commodity. Like other commodities, they are produced and sold by one group, purchased and consumed by another. In some cases a third party may participate, such as a distributor or clearing house, whose principal purpose is to facilitate commerce, but the principal parties remain the producer and consumer. The producer and consumer may work within the same organization, or indeed even be the same person, so the terms of the exchange of materials data may not always be apparent. But a producer of any commodity incurs costs in bringing that commodity to the marketplace. At a minimum, these costs must be met to assure solvency. The producers who prosper are those that excel not only in production but also in marketing.

This volume documents the proceedings of the Fourth International Symposium on the Computerization and Use of Materials Property Data, which was held at the National Institute of Standards and Technology (NIST) in October 1993, and sponsored jointly by ASTM Committee E49 on Computerization of Material and Chemical Property Data and NIST. The first two symposia in this series emphasized the production of materials data; the latter two focused more on the consumption of these data. There are many different kinds of consumers in the materials data marketplace, with varying needs and resources. Undoubtedly the customers with the most to gain from the successful use of materials data, and correspondingly the most to lose from the mis- or non-use of materials data, are those responsible for the design of capital structures, commercial/industrial equipment, consumer goods, and military hardware. It is with these users in mind that the symposium organizing committee invited Professor David Ullman to deliver a keynote address on "The Materials Selection Needs of Designers."

In his talk Ullman enumerated four types of materials selection assistance that designers typically seek:

1. Properties for specific material
2. Candidate material(s) for specific performance requirements
3. Comparison of current problem to existing case data
4. Automatic selection based on current knowledge

Specific needs of the design community identified by Ullman included:

- multiple levels of abstraction
- more stochastic information
- estimates/defaults where information is lacking
- integration into CAD and manufacturing process
- performance data, for example, fatigue, wear, corrosion, etc.
- cost/availability data
- improved access to information
- standards

Most of the papers in this volume address one or more of these types of material selection assistance and designer needs. The evolutionary nature of these needs, however, is apparent in Ullman's concluding statement: ''We do not have a good understanding of the information needed by designers. They are the customers of the database. Listen to your customers.'' This statement made on behalf of the users of materials data confirms their view of materials data as a commodity.

Many themes emerged during this symposium. The papers have been presented in this volume in groupings that reflect some of these themes.

Concurrent Engineering; Organization and Processing of Materials Data

In his paper, ''Common Data Processing Needs for Materials Databases,'' Nishijima discusses the benefits of fitting materials property data to models. The author then introduces the efforts under the Versailles Project on Advanced Materials and Standards and a Japanese standardization activity to develop a common data processing system. Finally, he demonstrates the advantage of utilizing such systems with examples on surface chemical analysis data and high temperature superconductor data.

In ''Data Management Demands of Complex Materials Models,'' King et al. propose a recursive structure to provide a more flexible and uniform data model. The authors describe the material state and process path model, underlying a materials property database for storage and retrieval of test data. They maintain that the role of the process path description inherent within the model is to identify appropriate assumptions for values of particular material properties for all subsequent material states of the process path.

In ''Integration of Test Methodology, Material Database, and Material Selection/Deselection Strategies for a Chemical-Material Compatibility Database System,'' Shuely describes a paperless process for transferring experimental data sets from instrumentation to a computer database. He also discusses the application of these methods to the selection of polymeric materials.

The last two papers in this first thematic group describe successful examples of the integration of materials data into the design process. In ''Space Transportation Main Engine Database Standardization'' Lee et al. describe a large, concurrent engineering data management procedure for developing a materials database in support of the space transportation main engine program. Mack et al. in ''Computerized Materials Data Integration in an Air Force Analytical Design Package,'' demonstrate the benefits of concurrent engineering and describe a computerized design tool for the loading, processing, cataloging, and transferring of data between various applications.

Database and Expert System Applications: Specific Materials

In ''Property Database on Shape Memory Alloys for Engineering Design,'' Tang and Sandström describe some of the unique properties of Ti-Ni, Cu-base, and Fe-base alloys with the ability to recall their shape in a previous state after a temperature or stress change. The authors also describe a database of properties of these materials. In ''Pavement Materials Property Databases for Pavement Management Applications,'' Uddin describes system design considerations and analysis requirements related to pavement material property database management. The paper also includes three case studies of pavement material database development.

In ''Advanced Composite Material Property Data Modeling for Engineering Analysis and Design,'' Spainhour et al. describe the development of a conceptual data model for fiberreinforced composite materials data. The authors illustrate basic elements of a composite materials database using diagrams that distill the information content down to the concepts of: entities or objects, relationships between those entities, and attributes or properties of the entities and relationships. The authors argue that the proposed model encompasses the data needs of engineers throughout the life cycle of a composite material component.

The last two papers in this grouping describe fledgling expert system development efforts. In ''The Role of Corrosion in a Material Selector Expert System for Advanced Structural Ceramics,'' Munro describes the development of a knowledge base for a material selector expert system based on relations among composition, microstructure, transport processes, operating conditions, and corrosion. The emphasis of the expert system is on the performance of ceramics at elevated temperatures. In ''Background and Basis for a Knowledge Elicitation Shell for Lifetime Predictions from Stress Corrosion Cracking Data,'' Roberge describes a software tool for the assessment of stress corrosion cracking occurrence for 7000 series aluminum alloys, based on the work of R. W. Staehle.

Strategic Use and Packaging of Existing Materials Data

The next two papers in this group describe excellent examples of the packaging and delivery of materials data. In ''Delivering Materials Engineering Information Using Hypermedia Systems,'' Arents et al. summarize hypermedia history and technology. The authors illustrate two hypermedia systems for navigation and retrieval of text, graphics, and photographic images: (1) a CD-rom based system that contains a diversity of corrosion-related information, and (2) an on-line client/server system providing information on the properties and characteristics of materials for use in solving materials engineering problems. In ''The Development of a Corporate Information Bank for Materials Data Using Commercial Available Software,'' Agema describes a materials information system incorporating property data, failure analysis reports, research results, and evaluation reports for use in the electricity generating industry.

In ''An Intelligent Object-Oriented Database System for Materials Information,'' Smith et al. describe a system incorporating a materials database, a knowledge base of geometric shapes, and a knowledge base of formulas, all in an object-oriented framework. The authors provide examples of how the system can be used to solve simple, quantitative problems and to select materials. They argue that systems which integrate materials information with knowledge on geometry and the laws of physics are inevitable.

Finally, in ''Review of Materials Property Relationships for Use in Computerized Life Assessment,'' Jaske discusses the material properties typically required for remaining-life predictions and how they should be interfaced with known life calculation algorithms.

Materials Data Applications of Emerging Information Technologies

In ''Neural Networks for Materials Data Analysis: Development Guidelines,'' Smets and Bogaerts summarize the technology of artificial neural networks. The authors provide many useful development guidelines and give examples in corrosion. They conclude that the technology is labor-intensive and that a good neural network model can only be found by trial-and-error.

In ''Database and Knowledge Acquisition for Ceramics Design,'' Xia et al. describe an advanced ceramics database and two separate knowledge acquisition efforts. The first effort was based on experience and resulted in a knowledge base on mechanical properties of zirconia ceramics. The second effort was based on experimental data and involved the use of neural networks for deriving rules from those data.

In "A Software Tool for Material Data Analysis and Property Prediction: CASAC-ANA," Zhou et al. describe three case studies of seven methods of material data analysis and property prediction. The authors emphasize the use of traditional statistical methods for data analysis. In addition, they describe their experience using emerging technologies such as artificial neural networks, and they also consider some lesser known techniques such as nonlinear mapping, hierarchical clustering analysis, etc.

Finally, in "Matching Information Technologies with the Objectives of Materials Data Users," Begley and Sturrock relate the principal themes of this thematic group back to the overriding theme of the symposium. The authors examine six information technologies: (1) expert systems, (2) multimedia, (3) object-oriented database management systems, (4) neural networks, (5) case-based reasoning, and (6) virtual reality. For each technology, they provide: (1) concepts and historical context, (2) illustrations of how these technologies have been and/or can be applied to benefit users of materials data, and (3) references of materials-related applications. The authors acknowledge the importance of standards organizations such as ASTM in providing robust guidelines for developers of materials data informatics that meet the needs of materials data users.

Opportunities and Outlook

In view of the preceding paragraphs it is evident that any supplier or consumer of materials data would find guidance within these pages. This book should be equally useful to anyone involved in the generation or development of materials data, as well as to those involved in design, manufacturing, processing, or other activity requiring the use of materials data. The broad, international scope of views expressed herein is particularly appropriate with the ever increasing globalization of both the economy in general, and the materials data marketplace in particular.

Much remains to be done, however, before we achieve market equilibrium. The standardization efforts are hard pressed to keep pace with rapid technological developments in packaging and delivery of materials data. As a result, there is still very little electronic exchange across materials data products. In this and in previous volumes of this series we have seen many excellent examples of materials property databases, expert systems, artificial neural networks, and other information technology applications. We have yet to learn of any measurable *impact* of these or any other systems. Finally, the legal issues involved with the misuse (or non-use) of materials property data have yet to be addressed, despite the specific call for papers in this area.

The future will continue to witness a burgeoning of materials data simultaneous with the continuing evolution of information technology. The level of participation at previous symposia in this series suggests a cyclical pattern to significant developments in this area with a period of about four years. Consider the number of papers by year of symposium:

Symposium year	*Number of papers in the STP*
1987	31
1989	20
1991	32
1993	19

If the cyclical pattern of the past continues into the future, many of the seeds of ideas planted or germinated at the 1993 symposium should bear fruit in 1995, at the Fifth

International Symposium on Computerization and Networking of Materials Property Data. We hope that this volume provides sufficient inspiration for those working with materials data to participate in future symposia and other ASTM Committee E49 activities.

C. P. Sturrock

E. F. Begley
National Institute of Standards and Technology
Gaithersburg, MD 20899;
symposium chairmen and editors.

Concurrent Engineering; Organization and Processing of Materials Data

Satoshi Nishijima[1]

Common Data Processing Needs for Materials Databases

REFERENCE: Nishijima, S., "**Common Data Processing Needs for Materials Databases,**" *Computerization and Networking of Materials Databases: Fourth Volume, ASTM STP 1257,* C. P. Sturrock and E. F. Begley, Eds., American Society for Testing and Materials, Philadelphia, 1995, pp. 9–19.

ABSTRACT: An international collaborative work known as VAMAS shows that the same set of factual materials data could result in totally different property values when the analysis model and computational method are different. The work is followed by a collection of models and methods for a wide range of materials properties, with the intention to provide a better awareness to the database builders and users.

Establishment of commonly accepted methods for handling fatigue and creep properties data is under way at the Iron and Steel Institute in Japan. This includes consensus formation among concerned experts for the development of common data processing software to be used in their database systems. Other examples show that the use of these common systems will enhance the further development and use of computerized materials property data.

KEYWORDS: materials databases, data analysis models, inventory, creep (materials), fatigue (materials), surface chemical analysis, high-temperature superconductors, common data processing, computers, data systems, computerized material property databases

In materials database systems that are oriented to scientists and engineers, there are often various subsystems allowing users to analyze retrieved data on materials properties. In the previous volumes of this symposium, many examples applying statistical treatments and some fitting analytical models to the data [*1–6*] can be found.

The present paper emphasizes the importance of analysis models and methods of materials data, and encourages database builders and users to develop common data processing systems that are based on accepted models and methods. This paper introduces the efforts under the umbrella of VAMAS (Versailles Project on Advanced Materials and Standards) [*7*] and a standardization activity to develop a common data processing system at the Iron and Steel Institute of Japan (ISIJ), and demonstrates the advantage of utilizing such common systems with examples on surface chemical analysis data and high temperature superconductor data.

Significance of Data Analysis Models

Unlike physical or chemical properties of substances, most engineering materials properties are defined as values generally deduced from test results obtained from accepted test methods. In the case of the tensile property of metallic materials, for example, the value is determined for standard specimens by standard test procedures, because it is dependent on such factors as specimen configuration, strain rate, etc. Many test methods are thereby

[1]Director, Failure Physics Division, National Research Institute for Metals, 1-2-1, Sengen, Tsukuba, Ibaraki 305, Japan.

standardized with specific data-deducing procedures of characteristic values, but there are still important materials properties that are not uniquely determined under actual situations.

This is often the case when the target property of a material is to be determined from a set of test data that might be retrieved from databases. In one of the frequent cases, the property value is estimated by interpolation or extrapolation of the data, or the property is represented by some parameters of a mathematical model fitted to the data. Long-time creep rupture strength at 100 000 h for heat-resisting alloys is a typical example of the former case, and the Weibull coefficient as a reliability index for engineering ceramics in the latter case.

Usually, long-time creep strength data are extrapolated from short-time data at higher temperatures, because long-time testing is difficult to conduct. The short-time data are evaluated by mathematical formulas that are based on theoretical or empirical models that are used commonly by special engineering groups. The problem is that there are several different models and processes for data treatment that give different property values to different people within their professional groups.

Generic Reasons for Fitting Materials Data to Models

Table 1 lists generic reasons why materials data are fitted to models. Prediction of a property value with confidence intervals is one of the most significant reasons in engineering design that the models and methods are needed. Disagreement in such values could be serious when the property is related to the reliability of materials, for example, the life or the strength to be referred to in a design. It may even give rise to a distrust of the materials database, because the data processing models and methods are incorporated normally in the database systems and the users would rely entirely on them without reflection.

VAMAS Round-Robin Comparison on Data Analysis Models

Problems due to discrepancies between the data analysis models and methods were revealed in a VAMAS workshop in 1988 and studied in a collaborative work [*8,9*]. A brief summary is presented here to show how significant differences can be produced from the same set of material data when analyzed with arbitrary models and methods.

The interpolation and extrapolation of experimental data are commonly used in the life assessment of materials for structural components, for example, for the fatigue or creep of metallic materials. In both cases, the basic materials life data are obtained generally from tests that are conducted at discrete stress values at fixed temperatures for relatively short times. However, the required materials behavior should cover any stress or temperature value in the form of continuous functions and for an extended time span: there is a substantial need for models that fit the data.

TABLE 1—*Needs of fitting materials property data to models.*

Catch general trend and scatter of the data
Evaluate quality of the data set
Deduce characteristic values of the property
Compare the data with other data (statistical tests)
Predict values by interpolation and extrapolation
Determine confidence limits of the property
Obtain mathematical expression for further uses

Property Data for the Round Robin

Several sets of creep and fatigue data were selected for this project, because it was thought that there were well-established analytical models and methods widely used in materials databases. The selected data consisted of four representative properties on six typical engineering materials, and was presented in pairs of well-balanced and ill-natured series. All the data were extracted from the Creep Data Sheets and Fatigue Data Sheets published by the National Research Institute for Metals (NRIM) of Japan.

The initial call for participation in the work was sent through contact persons of the VAMAS countries to experts on materials databases who are known to be experienced in the relevant data analyses. Because it resulted in many positive replies, copies of the full data set were distributed to each participant in a machine readable form to be analyzed by their own analysis models and methods.

Table 2 summarizes the combination of data sets for properties and materials, expressed with codes, and the number of reports submitted to NRIM from 15 participants from five countries. The number of substantially different models found in the reports are also listed in Table 2.

Findings from the Round-Robin Model Comparison

A complete analysis of results and discussions have been reported separately [*8,9*]. Here, only one result is shown for demonstration purposes, Fig. 1. It shows the result of fatigue life data analyzed with six different models by five experts from three countries. Note that the arrows on the right indicate the run-out or discontinued test data. It is astonishing that the deduced curves are so different. Apparently, there are three types of analysis models: simply excluding the run-outs, taking the run-outs as failed by engineering judgment, or including the run-outs by sophisticated statistical methods such as Probit analysis [*9*].

It is also noted that the result is dependent on the choice of objective and explaining the variables in the analysis. The life plotted on the abscissa is in fact the object of fatigue testing, while in engineering applications the strength along the ordinate is considered usually as the object to be explained by a function of the life. The choice of scales on coordinates, log-log or semi-log, can cause other differences in the results. The effect of these factors seems to be minor in magnitude but essential in practice.

Regarding the subject of the present paper, major conclusions from this collaborative work can be summarized as follows:

TABLE 2—*VAMAS round-robin comparison of data analysis models: codes for combinations of property and materials examined.*

Material Classes	Creep		Fatigue	
	Life	Strain	Life	Crack growth
Carbon steel	...	...	C-a	...
Low alloy steel	...	...	C-b	...
Welded joint	...	...	...	D-c
Low alloy steel	A-d	B-d	...	...
Stainless steel	A-e	B-e	...	...
Alloy steel	A-f	B-f	...	...
Number of reports	8	5	5	4
Number of models	11	6	8	4