

A Guide to Locating and Accessing Computerized Numeric Materials Databases*

E.F. Begley and S.J. Dapkunas

The widespread and rapid growth of materials research, together with the desire to shorten design times for commercial products, has increased the importance of numeric databases as ready sources of information. This article provides the materials engineer and component designer a guide to these sources including the data available and the points of contact for gaining access.

Keywords

materials databases, computerized numeric databases

1. Introduction

THE rapid and widespread development of new materials together with the increased use of computer-aided design (CAD) presents materials engineers and component designers with the daunting task of maintaining awareness of the availability of materials with unique properties as well as access to reliable property data. Historically, data for the more limited number of materials available were retained in manually accessed hard copy format such as handbooks, specifications, and codes. These factors and the necessity of gathering information rapidly to make concurrent engineering possible have encouraged the development of computerized databases. These databases are user friendly and contain reliable, evaluated data with sufficient detail to allow confident use. General familiarity with, and availability of, powerful personal computers has created an environment that encourages the routine application of these databases. Structural ceramics such as silicon nitride and silicon carbide exemplify materials with near-term application for which computerized evaluated databases of physical properties can be of use to engineers for both the selection of materials to satisfy known operating parameters as well as to establish designs based on properties of specific materials. It should also be noted that these databases allow rapid identification of gaps in the data, which can target research efforts early in the design process.

It is relatively straightforward to locate a handbook, because there are well-established points of entry to the world of printed material; libraries and compendiums of books in print are two such gateways. However, the world of computerized numeric materials databases is presently somewhat more enigmatic because it is less familiar and less mature, although both of these conditions are quickly improving. This guide will point the way to finding and accessing these specialized databases.

E.F. Begley and S.J. Dapkunas, National Institute of Standards and Technology, Ceramics Division, Gaithersburg, MD 20899.

*Certain commercial names are identified in this report for the purpose of clarity in the presentation. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology.

2. Scientific and Technical Data

Much effort has been given to categorizing scientific and technical data. Rumble and Smith^[1] provide the classification in Table 1. Others^[2,3] have extended this classification scheme to technical databases, wherein the combination of data types that comprise the database determines its category. In reality, technical databases are generally hybrids and contain several data types, but two broad categories are the most common for science and technology—bibliographic and numeric. Bibliographic databases contain citations and, often, abstracts for papers, reports, and dissertations that are related to a specific topic. Hightower and Schwarzwald^[4] give an excellent review of bibliographic materials science databases. Numeric databases contain primarily numbers such as those related to chemical or physical characterization and property measurements. Allan and Ferrell^[5] and the International Council for Scientific and Technical Information (ICSTI)^[6] survey numeric databases in science and technology.

In this guide, attention will be focused on numeric materials databases. Marginal effort has been made to establish the quality of the cited databases, and caution, as always, is urged when using data from these sources. Data quality is often reflected by the adequacy of the material specification, the sufficiency of the property test method descriptions, and qualification, preferably by an expert in the field, of the accuracy of the data values. Databases may vary in size, content, and availability, but data quality is a singularly critical issue in their development and use. Blind reliance on simple compilations of unevaluated data

Table 1 Primary types of technical data

Type	Description
Text	Names, words, and records using the 26 Latin letters plus punctuation and text layout
Numbers.....	Real, integer, error estimates, complex, imaginary
Scientific text.....	Names, words, records, and mathematics using Greek and other characters, superscripts and subscripts of all characters
Relationships	Equations and correlations
Rules	Interpretation and use, constraints, methods of application
Representational images	Chemical structure diagrams, graphics, diagrams, biological drawings
Pictures.....	Photographic images, halftones

encourages false confidence, leading to inappropriate use and faulty selection and design.

3. Sources of Computerized Numeric Materials Databases

Computerized numeric materials databases may be accessed through on-line systems or purchased. Thousands of such databases, whose topics range from planetary materials to welding electrodes, are available, and it would be inappropriate and impossible to tabulate all of them. Therefore, this article focuses on databases that are publicly accessible and produced in whole or in part in the United States.

3.1 On-Line Systems

On-line systems are those that are accessed via terminal or personal computer and modem and are offered primarily, but not exclusively, by information services. The services generally require users to pay certain fees, including account activation, telecommunications connection time, saved queries at the end of the month, and saved sets of retrieved records at the end of the month. To reduce costs, users should plan their searches carefully before connecting to these on-line services.

Four of the major commercial on-line services are:

- **BRS Information Technologies**
8000 Westpark Drive
McLean, VA 22102
Customer Service and Marketing: (800) 955-0906
General Information: (800) 289-4277
Local: (703) 442-0900
- **DIALOG Information Services, Inc.**
3460 Hillview Avenue
Palo Alto, CA 94304
Customer Service: (800) 334-2564
Local: (415) 858-3785
- **Orbit Search Service**
8000 Westpark Drive
McLean, VA 22102
Customer Service: (800) 456-7248
Local: (703) 442-0900
- **STN International**
2540 Olentangy River Road
P.O. Box 3012
Columbus, OH 43210-0012
Customer Service: (614) 447-3600

These companies provide catalogs describing the databases they offer, and often, there is overlap among services. The following are partial compendiums of numeric databases offered by each service.

BRS Information Technologies

Database Name: ELECTRONIC MATERIALS INFORMATION SYSTEM

Description: This database contains the latest data on properties of materials important in the fields of microelectronics and solid state research.

Producer(s): Institution of Electrical Engineers (INSPEC)

DIALOG Information Services, Inc.

Database Name: PLASPEC

Description: PLASPEC contains information on commercially available plastic materials including thermoplastic, thermoset, and elastomer products.

Producer(s): PLASPEC

ORBIT Search Service

Database Name: CORROSION

Description: CORROSION contains data on the effects of more than 600 corrosive agents on the most widely used structural metals, plastics, nonmetallics, and rubbers over a broad range of temperatures at controlled conditions. This database helps in solving existing corrosion problems, in selecting the best material of construction for a specific application cost and service life, in avoiding corrosion pitfalls, in determining the potential extent of corrosion problems, and in monitoring corrosion of existing systems and components.

Producer(s): ORBIT Search Service

Database Name: MDF/I

Description: MDF/I contains extensive numeric data for ferrous and nonferrous metals and alloys.

Producer(s): ASM International

STN International

STN International offers two databases of special importance, MPDSEARCH and NUMERIGUIDE. These will be described before the remaining STN selections.

Database Name: MPDSEARCH

Description: MPDSEARCH, the Materials Property Data Network, Inc. Guide to Materials and Substances Data Services, supplies information about the materials property databases available on STN International and the MPD Network. On-line and other computer-readable data sources for materials and substances property data, either publicly accessible or privately held, are included.

Producer(s): The National Materials Property Data Network, Inc. (MPD Network). Note: The MPD Network is available through STN International. For more information, contact:

The National Materials Property Data Network, Inc.
2540 Olentangy River Road
P.O. Box 02224
Columbus, OH 43202
(800) 848-6538 Ext. 3661 (USA and Canada)
(614) 447-3706 (all countries)

Database Name: NUMERIGUIDE

Description: This database is a data directory and property hierarchy file containing information on all the numeric properties available in each numeric database on STN International. NUMERIGUIDE includes appropriate terminology for each property, property definition, databases where the property may be searched, and default units for the property in each database. These properties may be searched either directly or via the accompanying thesaurus database.

Producer(s): The American Chemical Society

Database Name: ALUMINUM ASSOCIATION ALUMINUM STANDARDS AND DATA (AAASD)

Description: AAASD contains nominal composition and composition limits, mechanical and physical properties, and minimum tensile properties of commercial wrought aluminum alloys. AAASD is available through the MPD Network on STN.

Producer(s): Aluminum Association, Incorporated

Database Name: ALUMINUM FRACTURE TOUGHNESS DATABASE (ALFRAC)

Description: ALFRAC is a compilation of results of individual plane-strain fracture toughness and associated unevaluated notch-tensile test results for aluminum alloys. ALFRAC is available through the MPD Network on STN.

Producer(s): The Materials Properties Council, Inc., The Aluminum Association, Inc., and The National Institute of Standards and Technology

Database Name: COPPERDATA

Description: This database contains numeric data for physical and mechanical properties of copper and copper alloys. COPPERDATA is available through the MPD Network on STN.

Producer(s): Copper Development Association

Database Name: INTERNATIONAL PLASTICS SELECTOR (IPS)

Description: IPS contains manufacturer-supplied data on mechanical, thermal, electrical, and processing properties as well as flammability and uses for more than 12,000 commercial plastics. IPS is available through the MPD Network on STN.

Producer(s): International Plastics Selector, D.A.T.A. Business Publishing

Database Name: MARTUF

Description: This database contains the results of approximately 20,000 individual tests covering the toughness of steels identified as most important for marine applications by the Ship Structures Committee and the US Coast Guard. MARTUF is available through the MPD Network on STN.

Producer(s): Materials Properties Council

Database Name: MIL-HDBK-5 (MH5)

Description: MH5 contains numeric design, mechanical, and physical properties for metallic aerospace materials. MH5 is available through the MPD Network on STN.

Producer(s): US Department of Defense and Federal Aviation Administration

Database Name: STEELTUF

Description: STEELTUF includes numeric toughness data from more than 15,000 tests of steels for power and petroleum industry applications. The dominant type of data are Charpy notched bar impact energy along with tensile properties. STEELTUF is available through the MPD Network on STN.

Producer(s): Electric Power Research Institute (EPRI), The Materials Properties Council, Inc.

* * *

Some examples of on-line databases not offered by services follow:

Database Name: DIELECTRIC—EPRI DATABASE ON DIELECTRIC MATERIALS

Description: This database contains comprehensive property information on dielectric materials.

Producer(s): The Center for Information and Numerical Data Analysis and Synthesis (CINDAS)

Availability: For information contact:

CINDAS

Dr. C. Y. Ho

Purdue University

2595 Yeager Road

West Lafayette, IN 47906-1398

(317)494-9393

Database Name: MANLABS—NPL MATERIALS DATA BANK

Description: MANLABS contains thermochemical data on over 2000 materials including metals, inorganic compounds, alloys, and metals or gases in solution.

Producer(s): Manlabs

Availability: For information contact:

Manlabs

21 Erie Street

Cambridge, MA 02139

(617) 491-2900

Database Name: MAPTIS—MATERIALS & PROCESSES TECHNICAL INFORMATION SYSTEM

Description: MAPTIS is maintained by the NASA Marshall Space Flight Center for use by designers, contractors, materials engineers, NASA centers, and hardware developers. The system contains databases on atomic oxygen, thermal vacuum stability, metals, nonmetals, standard parts, plastics, nozzle materials, coatings, tapes, adhesives, and lubricants.

Producer(s): NASA

Availability: For information contact:

NASA

C.F. Key

Marshall Space Flight Center

Huntsville, AL 35812

(205) 544-2487

Database Name: RPDBC & SS

Description: RPDBC & SS is the Corps of Engineers repair products database for concrete and steel structures. It contains property data and end-use information for materials used in the repair and maintenance of concrete and steel structures.

Producer(s): CEWES-SC-CE

Availability: For information contact:

CEWES-SC-CE

Roy L. Campbell Sr.

3909 Halls Ferry Road

3.2 Databases That May Be Purchased

Database Name: CORROSION PERFORMANCE DATABASES

Description: COR*SUR 1 contains data for 25 common metals for exposures in over 1000 corrosive environments at various temperatures and concentrations. COR*SUR #2 provides similar data for 36 nonmetallic materials (elastomers, polymers, composites, thermoplastics, etc.) in over 850 environments.

Producer(s): National Association of Corrosion Engineers, Standard Reference Data at the National Institute of Standards and Technology

Availability: The CORROSION PERFORMANCE DATABASES run on IBM-compatible personal computers. These databases may be purchased from:

National Association of Corrosion Engineers
P.O. Box 218340
Houston, TX 77218
(713) 492-0535

Database Name: CHEMRESIST—CHEMICAL RESISTANCE OF PLASTICS

Description: CHEMRESIST contains test data on the effects of over 1600 chemicals on over 60 generic plastics.

Producer(s): Information Retrieval Systems

Availability: CHEMRESIST runs on IBM-compatible personal computers and is available from:

Information Retrieval Systems
Jay Parekh
1705 Second Avenue
Suite 3N
New York, NY 10128
(212) 348-6268

Database Name: COPPERSELECT—COPPER DEVELOPMENT ASSOCIATION DATABASE

Description: CopperSelect contains typical and minimal property values for commercial US copper and copper alloys, both cast and wrought. The database contains specifications, supplier information, applications, and processing characteristics as well as mechanical and electrical properties.

Producer(s): Copper Development Association

Availability: COPPERSELECT runs on IBM-compatible personal computers and is available from:

Copper Development Association
260 Madison Avenue
16th Floor
New York, NY 10016
(212) 251-7200

Database Name: NIST CRYSTAL DATA

Description: This database contains chemical, physical, and crystallographic information useful to characterize more than 154,000 inorganic and organic crystalline materials. The data include the standard cell parameters, cell volume, space group number and symbol, the calculated density, and classification

by chemical type, chemical formula, and chemical name. Each entry has an associated literature reference. Comprehensive chemical, crystallographic, and identification search software is provided with the database.

Producer(s): JCPDS—International Centre for Diffraction Data, Standard Reference Data at the National Institute of Standards and Technology

Availability: CRYSTAL DATA is available on magnetic tape and CD ROM. The database may be purchased from:

JCPDS—International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, PA 19073-3273
(215) 328-9400

Database Name: ELECTRON DIFFRACTION DATABASE

Description: This database is designed for phase characterization obtained by electron diffraction methods. The associated software permits very selective identification procedures for microscopic and macroscopic crystalline materials. The database contains chemical, physical, and crystallographic information on over 70,000 materials including minerals, metals, intermetallics, and general inorganic compounds. The data for each entry include the conventional cell, reduced cell, lattice type, space group, calculated or observed *d*-spacings, chemical name, chemical and empirical formula, material class indicators, references, and other parameters.

Producer(s): JCPDS—International Centre for Diffraction Data, Standard Reference Data at the National Institute of Standards and Technology

Availability: ELECTRON DIFFRACTION DATABASE is available on magnetic tape or CD ROM. The database may be purchased from:

JCPDS—International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, PA 19073-3273
(215) 328-9400

Database Name: Mat.DB

Description: Mat.DB is a database management system designed for maintaining information on the properties and processing of engineered materials. Data sets are available for alloy steels, aluminum, composites, copper, magnesium, nylons, stainless steels, structural steels, thermoplastics, thermosets, and titanium.

Producer(s): ASM International

Availability: Mat.DB runs on IBM-compatible personal computers and is available from:

ASM Center for Materials Data
Materials Park, OH 44073-0002
(800) 356-7538 Fax: (216) 564-7846

Database Name: NIST/SALTS—NIST MOLTEN SALTS DATABASE

Description: NIST/SALTS calculates property data on molten inorganic salts.

Producer(s): Molten Salts Data Center in the Chemistry Department at Rensselaer Polytechnic Institute

Availability: NIST/SALTS runs on IBM-compatible personal computers and is available from:

Standard Reference Data
National Institute of Standards and Technology
Building 221/Room A320
Gaithersburg, MD 20899
(301) 975-2208 Fax: (301) 926-0416

Database Name: PHASE DIAGRAMS FOR CERAMISTS DATABASE

Description: This database provides access to all diagrams from Volumes 6 to 8 in the well-known and widely distributed *Phase Diagrams for Ceramists* (PDFC). The software allows searches by chemical system, author, and year of publication. Diagrams may be plotted on-screen and the graphics software permits magnification of selected regions, overlay of related diagrams, lever rule calculations, display of the cursor position in real units, and selection of the temperature scale. Also, all bibliographic references and chemical systems from Volumes 1 to 8 of the PDFC series are available.

Producer(s): American Ceramic Society, Standard Reference Data at the National Institute of Standards and Technology

Availability: The PHASE DIAGRAM FOR CERAMISTS DATABASE runs on IBM-compatible personal computers and is available from:

The American Ceramic Society Book Sales Department
735 Ceramic Place
Westerville, OH 43081
(614) 794-5860

Database Name: STRUCTURAL CERAMICS DATABASE (SCD)

Description: This database contains thermal, mechanical, and corrosion properties of silicon carbides and silicon nitrides. The SCD also contains a bibliography with complete documentation of data sources through 1991.

Producer(s): Gas Research Institute, Standard Reference Data at the National Institute of Standards and Technology

Availability: The STRUCTURAL CERAMICS DATABASE runs on an IBM-compatible personal computer or on a Macintosh with PC emulator software. The database may be purchased from:

Standard Reference Data
National Institute of Standards and Technology
Building 221/Room A320
Gaithersburg, MD 20899
(301) 975-2208 Fax: (301) 926-0416

Database Name: TRIBOMATERIALS I (ACTIS) DATABASE

Description: This database contains property data for 261 materials commonly used in tribology applications. The data cover a range of properties including basic physical and mechanical as well as tribology properties for both lubricated and unlubricated wear.

Producer(s): ACTIS Inc., Standard Reference Data at the National Institute of Standards and Technology

Availability: The TRIBOMATERIALS I (ACTIS) DATABASE runs on IBM-compatible personal computers and is available from:

ACTIS
1118 Highgate Road
Wilmington, DE 19808
(302) 998-8240

Database Name: X-RAY PHOTOELECTRON SPECTROSCOPY DATABASE

Description: This database provides access to photoelectron and Auger spectral data and contains over 13,000 line positions, chemical shifts, and splittings. Each record in the database supplies:

- Element and chemical compound, including names and formulas
- Line type, i.e., photoelectron, Auger, Auger parameter, chemical shift, doublet splitting, other splittings
- Line energy or energy difference
- Experimental details such as calibration, charge reference, and physical state
- Reference citation

Producer(s): Standard Reference Data at the National Institute of Standards and Technology

Availability: The X-RAY PHOTOELECTRON SPECTROSCOPY DATABASE runs on an IBM-compatible personal computer or on a Macintosh with PC emulator software. The database may be purchased from:

Standard Reference Data
National Institute of Standards and Technology
Building 221/Room A320
Gaithersburg, MD 20899
(301) 975-2208 Fax: (301) 926-0416

4. Conclusion

There is no one source of computerized numeric materials databases. Systems are constantly being developed by private individuals, university departments, corporations, and government agencies. This guide supplies information that should help direct researchers and engineers toward the databases they need. MPDSEARCH is perhaps the most comprehensive database on numeric materials databases and includes international listings that were beyond the scope of this article. Government agencies are also very active in the development and dissemination of computerized numeric materials data, although use of these databases can be restricted in various ways. Additional information is available from the following agencies:

Defense Technical Information Center
United States Department of Defense
The Pentagon
Washington, DC 20301-8000
(703) 274-6800
Scientific and Technical Information Office
United States Department of Energy
Oak Ridge, TN 37831

(615) 576-1188
Scientific and Technical Information Center
United States Department of Commerce
2231 Crystal Drive
Arlington, VA 22202
(703) 308-0808

National Technical Information Service (NTIS)
5285 Port Royal Road
Springfield, VA 22161
(703) 487-4929

References

1. J.R. Rumble and F.J. Smith, *Database Systems in Science and Engineering*, IOP Publishing Ltd., Bristol, England, 1990, p 8-9
2. A. Shoshani, F. Olken, and H. Wong, "Data Management Perspective of Scientific Data," *The Role of Data in Scientific Progress*, Proc. 9th CODATA Conf., P. Glaeser, Ed., North-Holland, Amsterdam, 1985
3. M.E. Williams, Ed., *Computer Readable Databases, Vol I, Science, Technology, Medicine*, Elsevier Science Publishing, 1985, p vii-viii
4. C. Hightower and R. Schwarzwald, A Comprehensive Look at Materials Science Databases, *Database*, Vol 14 (No. 2), 1991, p 42-53
5. F.C. Allan and W.R. Ferrell, Numeric Databases in Science and Technology: An Overview, *Database*, Vol 12 (No. 3), 1989, p 50-58
6. *Numeric Databases: A Directory*, International Council for Scientific and Technical Information (ICSTI), Paris, 1991