

MATERIALS DATA ON THE INTERNET

J. H. Westbrook

Brookline Technologies, 5 Brookline Road, Ballston Spa, NY 12020, USA

Email: jackwestbrook@earthlink.net

Abstract

The availability of the Internet has provided unprecedented opportunities for both data compilers and users. With respect to materials data, this paper explores: how do we know what is available? how can data be accessed, interpreted, exchanged? what novel modes of presentation are now available? what organizations are active in this field and what are their programs? what improvements are needed? where do we go from here and how? Examples will be illustrated of specific materials databases available on the Internet from a variety of materials data fields, e.g. fundamental data, engineering design properties, environmental data, and materials safety data. While there is no question that large and widely varied bodies of data are accessible on the Internet, significant improvements are needed promptly. The paper concludes by summarizing these problems and possible means for their alleviation-

Keywords: Data, Database, Engineering, Internet, Materials, Science

1 INTRODUCTION

Online materials data, available via the Internet, can serve several different purposes: materials selection, component/product design, design of materials, and risk management among others. While there are many databases now available, a comprehensive, mutually compatible set or informal system conforming to the best standards does not yet exist. This paper will review the present state of the field, highlight its achievements and shortcomings, and suggest some beneficial future actions.

2 AVAILABLE ONLINE RESOURCES

This is not the first time that an attempt has been made to survey materials data sources on the Internet. CODATA itself in 1993 produced a second edition of its "International Register of Materials Database Managers" (Barrett, 1993) and listed almost 200 databases. Meltsner (1995) provided a useful overview to materials science and engineering on the Internet. Ericsson (1998) posted his graduation thesis, "Materials Information on the Internet", containing ~200 site links, well classified and individually annotated. Westbrook (2002) published "Intermetallics on the Internet", which, while somewhat narrowly focussed, nonetheless included much of general interest to materials scientists and engineers, e.g. the search process, assists to searching, examples of useful sites and interesting results. Despite these efforts, there is still no truly comprehensive listing, printed or online, of recommended accessible sites on the Internet for materials data.

In attacking this problem there are two approaches to be considered: the use of directories and locators and the use of search engines. Printed directories to science and technology on the Internet exist including: Clement (1996), Hu, Xiau, & Zhang (1998), Renehan (1993), and Thomas (1998). Unfortunately, they are of limited utility for the present purpose: coverage of materials sources is scanty, and they quickly go out-of-date. Online directories are broad in scope and intrinsically current, at least potentially, but they have problems of their own. Some of the materials properties directories available on the Internet are listed in Table 1. Seeking such directories is made difficult by more generic use of the term *materials* (e.g. teaching materials) or by some alternative, non-relevant implication of the term *properties* (e.g. real estate). Search engines pose similar problems. Use of a search strategy ("data OR database OR databank" AND "materials") can readily yield millions of hits, and even specifying a particular materials class and properties class can still result in a hit list of tens of thousands. In order to restrict hits to sites containing

data that can be read on-screen and to avoid hits to isolated papers, books, bibliographies, CDs or other offline electronic files, conference proceedings, etc., other measures must be taken. The most effective path found is to preface the search with the term “online”. Thus using the Google search engine, the term “online” gives 180 million hits; searching within these using “materials” gives 4.05 million hits; and within this subset using “properties” 595 thousand hits. Yet searching within the last subset using “data OR database OR databank” finally focuses on 194,000 sites. The Yahoo and Ixquick engines produced similar results. All of these engines present their findings with the most important sites listed first, which is a help. To further narrow the list with any of these engines, it is necessary to specify a materials class or property group. Despite these difficulties in winnowing wheat from the chaff for materials data in a broad sense, the better search engines have no difficulty in locating a particular property of a specific material, e.g. the Néel temperature of magnetite. Using just these two terms, a search leads to a sufficiently small number of hits (34) that it is feasible to scroll through these and find one that contains the answer sought (578°C).

There are also sites that focus on a particular kind of data (see further below), and direct access to these may be more efficient than use of a search engine. For example, suppose one wishes to compare some basic properties of the refractory metals Cr, Mo, and W. By query of a periodic table site (e.g. that of the University of Sheffield, <http://www.webelements.com>) and clicking on each element in turn, such properties as atomic number, atomic weight, bulk properties, crystal structure, etc. are presented. If a particular phase diagram is needed, for example for the binary system Hf-Si, go to Georgia Tech’s site (http://www.cyberbuzz.gatech.edu/asm-tms/phase_diagrams/), click on one of the two component elements, then the other, and the selected diagram appears.

Somewhat akin to directories are so-called *metasites*, or focussed directories that gather together Uniform Resource Locators (URLs) and brief descriptions of sites with a common theme. As shown in Table 2 listing some materials-related instances, such themes may be disciplinary, institutional, application-oriented, or topical. The listings of Table 2 are representative, not exhaustive. The reader is also cautioned that while such metasites may list or even provide direct linkage to the sites they cover, access to the content of some sites may require a paid subscription or other fee. Although no truly comprehensive directory or listing of online materials databases yet exists, it is estimated that there are probably several hundred identifiable unique sites that provide reasonably broad coverage of materials properties.

As is obvious from the listings of directories and metasites in Tables 1 and 2, many different groups have been involved in building and maintaining materials databases. Each group has its own biases and slant on the provision of information. In the commercial category (e.g. MatWeb, MDI, CES Materials Data, ILI, Master Miner, MSC.Mvision....) the database builders are primarily interested in selling, either the information itself or the material to which it relates. Educational institutions (e.g. Indiana University, Massachusetts Institute of Technology (MIT), Rensselaer Polytechnic Institute (RPI), Edinburgh University, Kyoto University,.....) build their systems primarily to satisfy the information needs of their staff and students, but may as a courtesy offer access to anyone, free or for a modest fee. The institutional group which includes both government-affiliated (e.g. National Institute of Standards and Technology (NIST), National Institute of Materials Science (Japan) (NIMS), Versailles project on Advanced Materials and Standards (VAMAS), Naval Research Laboratory, European Community Joint Research Centers....) and professional (e.g. ASM International, American Society for Testing and Materials (ASTM), American Ceramic Society, ...), aim primarily to serve their constituencies but have no particular focus on any group of materials or class of properties. The result of this diverse sponsorship has been incomplete coverage with respect to both materials and properties, lack of standards for data representation and quality assessment, and difficulties in data exchange.

These problems have long been recognized, and 10 years ago several groups, - ASTM’s Committee E49 (Newton, 1993); CODATA’s Task Group on Materials Data Management (Barrett, 1993); and the International Standards Organization (ISO) (Rumble, 1992) - were active in promoting the subject and in improving both materials database building and access. Alas, neither of the first two named is active anymore. The ISO group, Technical Committee 184 (TC184/SC4), with inputs from the world’s largest industrial nations and many of their largest manufacturing companies, after 10 years of study, produced by 1994, ISO 13030, the STandard for the Exchange of Product Model Data (STEP) (Rumble, 1992). It is designed to support data exchange between software that performs all engineering functions associated

with manufactured products. While the STEP standard allows for a description of a materials product and its properties, it does so in a highly abstract form. Actual use depends on the formulation of a more specific information model set, an Application Protocol that captures the specific engineering requirements that are implementable in engineering software. This in turn requires populating the Protocol itself with data values or providing access to a persistent source such as a materials database via a standard access interface. Full implementation of this approach has yet to be achieved, particularly in the materials sector; some of the reasons for which are discussed by Swindells (2002). In a final instance, a National Materials Property Data Network (Kaufman, 1992), funded by the Chemical Abstracts Service and an industrial consortium, was established in 1991 following pilot studies of several years' duration in the late 1980s. Unfortunately, despite a common mode of access to about 10 individual databases and many supporting programs for search, display, and interpretation, MPDN folded by late 1993. Its demise has been attributed to insufficient funding and inadequate user friendliness.

There are, however, a few relevant projects that are current:

- The World-Wide-Web Consortium (W3C, n.d.), comprised of 500 member organizations, aims to promote interoperability, improve access in the semantic sense, and guide development of the Web. It has, however, no particular focus on materials.
- The NIST effort on Materials Markup Language (MatML), a materials adaptation of an extensible markup language (XML) for management and exchange of data (Murray-Rust and Rzepa, 2002). The current status of the MatML project is described by Sturrock and Begley (2002) and Begley and Sturrock (2002).
- A Materials Data Management Consortium (MDMC) has been established under the leadership of ASM International, Granta Design, Ltd., and the Life Prediction Branch of NASA's Glenn Research Center. Their goals are to save time and money and increase competitiveness by increasing the quality and traceability of materials data and by increasing the efficiency of materials data management and manipulation within each member organization.
- ASM International has long been a leader in data compilation and provision of access to reliable data on materials. It has a standing committee on Materials Properties Databases which advises the Society on print and electronic data publications and on data-related technical programming. It is now working on a Directory of Databases, which would presumably be published in *Advanced Materials and Processes* when completed. The Committee is reviewing the current set of 232 records, adding to them, eliminating those with no data at all that are simply promotional pitches for the materials producer or information vendor, and adding a quality index. ASM is currently collaborating with Granta Design, Ltd. of the UK on both CDs and other electronic products derived from ASM print publications and on online access to the 21 volume *ASM Handbook* and to the *Alloy Digest* data sheets. It also sells both print and downloadable PDF files of materials standards from other organizations, e.g. Institution of Electrical and Electronics Engineers (IEEE) and American Petroleum Institute (API).

It is also encouraging to note that the recently released National Materials Advisory Board (NMAB) Report, "Materials Research to Meet 21st Century Defense Needs", (Schadler, Lovelace, Baskerville, Capasso, Firebaugh, Gassner, Jaffe, Karasz, Lipsitt, Meyappan, Peterson, Phillips, & Tressler, 2003) made as one of its chief recommendations the establishment of a centralized database of materials and their properties, primarily to facilitate the more rapid introduction of newly invented materials into practical service.

3 PRINT REFERENCES TO ONLINE SOURCES AND COMPUTERIZATION OF MATERIALS DATA

In order to develop a more complete and current picture of the state-of-the-art with regard to the building, use, and analysis of computerized materials databases as well as to aid in further identification of and reference to such bases, it is desirable to cite some of the recent literature. With reference to the second point, Wawrousek, Westbrook, and Grattidge (1989) published an extensive listing and description of 1250 data sources on engineering materials which included about 140 computerized sources (not necessarily online). Each source was located in several of about 1100 cells of a materials/properties matrix so that it was possible for the user, by specifying a material class and property class, to quickly locate sources of possible interest. A brief, but more accessible, description of this project has also been published (Wawrousek, Westbrook, & Grattidge, 1991).

Every two years from 1987 to 1995 ASTM sponsored an international conference “Computerization and Networking of Materials Databases”, the proceedings of which are available in print. (Glazman & Rumble, 1989; Kaufman & Glazman, 1991; Barry & Reynard, 1992; Sturrock & Begley, 1995; Nishijima & Iwata, 1997). These proceedings record the progress that has been made over the years and highlight contributions from all over the world. Unfortunately, the series has not been continued.

Westbrook and Kaufman (1996) at an earlier CODATA meeting presented a brief but comprehensive review of impediments hindering the realization of facile access to data on engineering materials. They covered technical issues, economic and other non-technical issues, and content-related issues such as inadequacies in comprehensiveness, standardization, and quality and reliability.

Doyama, Suzuki, Kihara, and Yamamoto (1991) edited the proceedings of a 1990 Conference on Computer Aided Innovation of New Materials. The almost 200 papers from 19 different countries covered many different aspects of the location and utilization of properties data for a wide variety of materials and of the application of such to the modeling and simulation of both materials structure and processing. A sequel of the same scope and character was later published (Doyama, Kihara, Tanaka, & Yamamoto, 1993).

King and Monma (1995) have developed an inventory of available databases covering both physical and chemical properties.

Volume 20 of the *ASM Handbook* on Materials Selection and Design (Dieter, 1997) included 9 articles on the process of materials selection, 8 other articles on the effects of composition, processing, and structure on materials properties and a separate article (Westbrook, 1997) on materials property data and information (both print and computer-accessible) that treated the needs for such data, specific sources of data, and the evaluation and interpretation of the data.

4 INTERPRETATION OF THE NUMBERS

Having located a site containing some numerical data, the prospective user is confronted with several important questions: what is the provenance of these numbers? what is their significance? are they: min or max values, typical values, numbers with associated range limits or uncertainty parameters, experimental observations, theoretical estimates, or what? has their reliability or validity been checked and, if so, by whom and how?

Unfortunately, many existing online materials databases are silent on some or all of these questions. Granta Design (2002) has recommended a “zero order” approach to data checking that can at least catch most instances of incorrect entry, units confusion, or major inaccuracy in the original obtention of the datum. They recommend checking of the property value of interest against known ranges for various materials classes, subclasses, etc. and also checking such values against established property correlations, empirical or theoretical. Again, only in exceptional cases have such screenings been performed in the past

on materials data before presenting them online. In connection with the work of ASM's Committee on Materials Property Data, Kaufman (private communication, 25 Sept 2002) has proposed that each database considered for inclusion in ASM's Directory be rated according to three parameters: breadth of coverage with regard to specific numeric data; quality of data presented; and ease of access and searchability. For each category the database is to be rated 1 (highest) to 3 (lowest). This system has recently been formally adopted and should add to the utility of and confidence in this directory. NIST has developed a recommended practice guide (Munro, 2003) for evaluation of materials properties that addresses, from both theoretical and practical viewpoints, accessibility, responsibility, consistency, and predictability.

Another issue is the adequacy of the metadata presented with the data values shown in a materials database. Metadata have been defined as "data about data" and comprise the vital additional information about the material, property, data source, independent variables, units, test description, etc. associated with a given numerical datum. Westbrook and Grattidge (1991) have reviewed the metadata issues involved in building and using materials databases. Although this and similar references are more than 10 years old, the recommendations are still ignored. Some actual instances whose source (out of kindness) will *not* be cited follow: the temperature dependence of specific heat is reported to four significant figures, but the material which was tested is described only as "copper"; a figure of 20,000 psi is given for the creep strength of A286 alloy, but nothing is said of the state of heat treatment of the material, nor the temperature, strain, or time pertinent to the test conducted. Under such circumstances possibly useful data can neither be used, interpreted nor exchanged. Further examples of how omission of metadata has led to problems in the computerization of a classic printed materials data reference may be found in Grattidge, Lund, and Westbrook (1992).

5 DATA HANDLING

There is a wide variety of software available, both integrated multi-functional programs and dedicated single-purpose programs to harmonize, exchange, offer alternative presentation modes, perform calculations, convert units, etc. To fully explore this topic would require a separate paper. Here we will only present a few examples, especially pertinent to materials data.

MSIT – Connect (<http://www.msiwp.com/products>) is the interface to the MSIT[®]Workplace hosted at <http://www.matport.com>. It includes an interactive graphics package applicable to phase diagrams. Most of the phase diagrams, both binary and ternary, available through Materials Science International (Stuttgart) (MSI) have been digitized and are in a vector graphics format. Therefore zooming in on a particular portion of a diagram, changes in color or scale (atomic or weight percent), overlaying of diagrams, or extraction of coordinates of particular points of interest are all options available to the user.

Some of the crystallographic sites (e.g. <http://www.iumsc.indiana.edu> and Fachinformationszentrum's (FIZ, Karlsruhe) Crystal Visualizer (CVIS)) offer alternative pictorial presentations of the unit cell, rotation of a crystal model just as if it were in the user's hand to see relations between different crystallographic planes, etc.

TIMS: Tool for the Interpretation of Mass Spectra (<http://beelzebub.ethz.ch/Tbres.html>) A simple, freely downloadable, Mac tool for aid in the interpretation of mass spectra. Given an experimental mass spectrum and a possible structure, TIMS calculates all possible fragments obtained on removing one or two bonds.

MAP (<http://www.msm.cam.ac.uk/map/data/data-index.html>) This site provides neural network models (and the necessary data): to predict lattice mismatch of Ni-based superalloys, to calculate Ms temperatures for steels of arbitrary composition, to analyze solidification cracking of welds, and to study weld toughness.

For unit conversion see <http://www.conversion.com> 5000 units, 30,000 conversions, e.g. length, temperature, speed, volume, energy, pressure, viscosity, torque, etc.

MatHub (<http://www.mathub.com>) A site posted by Accelrys, Inc., a subsidiary of Pharmacoepia Inc., focuses on computational materials science on the web including modeling, a software directory, a 1500-item bibliography, knowledge management, and other aspects of materials information.

A Finnish site (<http://www.castech.fi>) offers a family of programs for simulation of the solidification of castings.

Information Technology Toolbox (<http://database.ittoolbox.com>) consists of an extended package of software tools for analyzing, normalizing, and presenting data together with online or referenced tutorials on the subject.

NIMS (Japan) (http://inaba.nims.go.jp/netnavi/link_F0831.htm) is an example of a materials information site designed to be multi-functional in that it provides not only its own data, but links to other sites, search engines, physical constants, unit conversion programs, the periodic table, modeling software, standards, etc., all at a single site.

A site similar to that of NIMS is Martindale's Reference Desk (<http://www.sci.lib.lib.uci.edu/HSG/GradMaterial.html>). Their "Virtual" Science Center provides language dictionaries, measurement data, periodic tables,, physical properties databases, chemical and biological databases, materials science databases, glossaries, and much else.

We conclude this section with brief descriptions of two unusual sites, each with a broad variety of information and unusual search capabilities.

MatWeb (<http://www.mymatweb.com>). This site, built by Automation Creations, Inc., provides properties data for about 28,500 materials! The user may search by materials type, by property, composition, manufacturer, trade name, Unified Numbering System number, etc. Polymers, ferrous metals, nonferrous metals, superalloys, pure elements, ceramics and other engineering materials are all covered.

Knovel (<http://www.knovel.com>). Knovel is an Internet search and retrieval subscription service providing online access to over 500 printed titles – handbooks, databases, and conference proceedings – in 15 technical subject areas, many of which relate to materials. Textual and database components of interactive databooks are searchable seamlessly and simultaneously by two search engines: database and full text. Interactive elements are not only field searchable using keyword and numeric searches, but also can be manipulated in many ways in the browse mode, using sort, select and find functionalities. The search is robust and involves Booleans, proximities, wild cards, variable units of measurements and nested queries. In addition, knovel has developed various calculation packages that are integrated with information extracted from books and databases. These include applets for digitization of graphs, comparison of curves from different graphs, function plotting and calculation.

A final aspect of data handling that must be mentioned is data mining, i.e. finding patterns, groups, clusters, and relationships in a large body of data. As an example of data mining in the materials field, we cite the work of Villars, Bradenburg, Berndt, LeClair, Jackson, Pao, Igel'nik, Oxley, Bakshi, Chen, and Iwata, (2000), who showed that a non-linear expression involving but a single material parameter, the Mendeleev number, could successfully account for the occurrence or non-occurrence of a ternary compound based on analysis of almost 7000 experimentally-determined metallic systems. An excellent introduction to data mining in general is the text by Han and Kamber (2000).

6 CONCLUSIONS

While there is no question that large and widely varied bodies of materials data are accessible on the Internet, significant improvements in both presentation and access are needed promptly, or else prospective users may become so frustrated and disillusioned that they abandon electronic access for data.

Among the problems that need to be addressed are:

- *A well-structured online directory to reliable materials data sources should be built.*
Existing directories are: incomplete, mix bibliographic and other information sources with numeric data, and exhibit considerable diversity in the reliability of the sources, completeness of meta-data, etc.
- *Persons or organizations posting data on an online site need to be encouraged to include detailed instructions for searching for and retrieving data.*
A title and the URL of the homepage are not usually sufficient. Many sites mix numeric data with other information, each site requires a different path to get to the numeric data contained, and subsequently different procedures must be followed to get to a particular property of a particular material.
- *Any online data site must make clear the provenance of the data shown.*
The provenance may be either categorical (e.g. manufacturer's data, specified by a recognized standard, experimental, theoretically predicted, etc.) or specific (where a literature citation or link to another online site must be provided).
- *Any data shown should be accompanied by full metadata for both the material whose properties are shown and for the property data themselves.*
Failing this, the user may retrieve data that are meaningless or misapply them to his problem.
- *Standardization of materials databases and means of access to them must be undertaken by recognized national or international bodies, government or professional materials databases.*
Only when such standards exist and are well publicized will even voluntary compliance occur and the user problems outlined here be alleviated.

Development of solutions to these problems are activities well within the purview of CODATA. Unfortunately, a materials-oriented task group no longer exists.

7 ACKNOWLEDGMENT

G. Effenberg, S.I. Gurke, S. Iwata, J.G. Kaufman, and P.J. Lindstrom are thanked for their helpful comments on an early draft.

8 REFERENCES

- Barrett, A.J. (Ed.) (1993) *International Register of Materials Database Managers, Special Report No. 14* (2nd ed.). Paris: CODATA.
- Barry, T.I. & Reynard, K.W. (Eds.) (1992) *Computerization and Networking of Materials Databases, STP 1140* (Vol. 3). Philadelphia: American Society for Testing and Materials.
- Begley, E.F. & Sturrock, C. (2002) The Background and Development of MatML, a Markup Language for Materials Property Data, Paper IV-A-1, #4 at Montreal CODATA Conf.
- Clement, G.P., Ed. (1996) *Science and Technology on the Internet: An Instructional Guide (Internet Workshop Series, No. 4)*. Berkeley, CA: Library Solutions Inst. and Press.
- Dieter, G.E. (Ed.) (1997), *Materials Selection and Design. ASM Handbook* (Vol.20). Materials Park, OH: ASM International.

- Doyama, M., Suzuki, T., Kihara, J., & Yamamoto, R. (Eds.) (1991) *Computer Aided Innovation of New Materials*. Amsterdam: Elsevier.
- Doyama, M., Kihara, J., Tanaka, M., & Yamamoto, R. (Eds.) (1993) *Computer Aided Innovation of New Materials, II*. Amsterdam: Elsevier.
- Ericsson, M. (1998) *Materials Information on the Internet*. [Thesis] Royal Institute of Technology, Sweden; contact: matser@material.kth.se.
- Glazman, J.S. & Rumble, J.R. (Eds.) (1989) *Computerization and Networking of Materials Databases, STP 1017* (Vol. 1). Philadelphia: ASTM.
- Granta Design, Ltd. (2002) Data Checking and Estimation. Retrieved Sept 1, 2002 from the Granta Design website: (<http://www.grantadesign.com/resources/tutorials/datachecking.htm>).
- Grattidge, W., Lund, W. B., & Westbrook, J.H. (1992) Problems of Interpretation and Representation in the Computerization of a Printed Reference Work on Materials Data. In Barry, T.I. & Reynard, K.W. (Eds.) *Computerization and Networking of Materials Databases, Vol.3*, STP 1140. Philadelphia: American Society for Testing and Materials.
- Han, J.-W. & Kamber, M. (2000) *Data Mining: Concepts and Techniques*. San Francisco, CA: Morgan Kaufmann.
- Hu, Y., Xiau, Y., & Zhang, H. (1998) *Resources Handbook of Science and Technology on the Web*, (Chinese and English). Beijing: People's Post & Telecommunications Publishing House.
- Kaufman, J.G. & Glazman, J.S. (Eds.) (1991) *Computerization and Networking of Materials Databases, STP 1106* (Vol. 2). Philadelphia: American Society for Testing and Materials.
- Kaufman, J.G. (1992) Online Access to Worldwide Sources of Materials Performance Data – 1991 Update on the Materials Property Data Network (MPD Network). In Barry, T.I. & Reynard, K.W. (Eds.) *Computerization and Networking of Materials Databases, STP 1140* (Vol. 3). Philadelphia: American Society for Testing and Materials.
- King, T.M & Monma, Y. (1995) Inventory of Material/Chemical Property Databases on Physical and Engineering Properties. *5th International Symposium on Computerization and Networking of Materials Property Data*, Tsukuba City, Japan.
- Meltsner, K.J. (1995) Understanding the INTERNET: A Guide for Materials Scientists and Engineers, *J. Metals*, 47 (4), 9-15.
- Munro, R.G. (2003) *Data Evaluation Theory and Practice for Materials Properties*, NIST Special Publication, 960-11, Washington, DC: National Institute of Standards and Technology.
- Murray-Rust, P. & Rezpa, H.S. (2002) Scientific Publications in XML – Towards a Global Knowledge Base, *Data Science Journal* 1 (1) 84-98.
- Newton, C.H. (Ed.) (1993) *Manual on Building of Materials Databases, MNL 19*. Philadelphia: American Society for Testing and Materials.
- Nishijima, S. & Iwata, S. (Eds.) (1997) *Computerization and Networking of Materials Databases, STP 1311* (Vol.5). West Conshohocken, PA: American Society for Testing and Materials.
- Renehan, E. (2000) *Scientific American Guide to Science on the Internet*. New York: ibooks.

- Rumble, J.R., Jr. (1992) The STEP Model of Materials Information. In Barry, T.I., & Reynard, K.W. (Eds.), *Computerization and Networking of Materials Databases*, (Vol. 3, pp. 141-149) STP 1140. Philadelphia: American Society for Testing and Materials.
- Schadler, H.W., Lovelace, A., Baskerville, J., Capasso, F., Firebaugh, M., Gassner, J., Jaffe, M., Karasz, F., Lipsitt, H.A., Meyappan, M., Peterson, G., Phillip, J.M. & Tressler, R. (2002) *Materials Research to Meet 21st Century Defense Needs, National Materials Advisory Board Report 498*. Washington, DC: National Academies Press.
- Sturrock, C.P. & Begley, E.F. (Eds.) (1995) *Computerization and Networking of Materials Databases, STP 1257* (Vol.4). Philadelphia: American Society for Testing and Materials.
- Sturrock, C. & Begley, E.F., (2002) MatML: A New Language for Materials Property Exchange over the Web, *AMPTIAC Quarterly* 6 (3) 7-9.
- Swindells, N. (2002) Communicating Materials Information: Product Data Technology for Materials, *International Materials Reviews* 47, 31-46.
- Thomas, B.J. (1998) *The WorldWide Web for Scientists and Engineers*. New York: American Society of Mechanical Engineers.
- Villars, P., Brandenburg, K., Berndt, M., LeClair, S., Jackson, A., Pao, Y.-H., Igel'nik, B., Oxley, M., Bakshi, B., Chen, P., & Iwata, S. (2000) Interplay of large materials databases, semi-empirical methods, neuro-computing and first principle calculations for ternary compound former/nonformer prediction, *Engineering Applications of Artificial Intelligence*, 13, 497-505.
- Wawrousek, H., Westbrook, J.H., & Grattidge, W. (1989) Data Sources of Mechanical and Physical Properties of Engineering Materials. *Physik Daten, No. 30-1*, Karlsruhe, Germany: Fachinformationszentrum.
- Wawrousek, H., Westbrook, J.H and Grattidge, W. (1991) Data Sources of Mechanical and Physical Properties of Engineering Materials. In Kaufman, J.G. & Glazman, J.S. (Eds.) *Computerization and Networking of Materials Databases, STP 1106* (Vol. 2). Philadelphia: American Society for Testing and Materials.
- Westbrook, J.H. (1997) Sources of Materials Property Data and Information, In *ASM Handbook* (Vol. 20, pp 491-506). Materials Park, OH: ASM International.
- Westbrook, J.H. (2002) Intermetallics on the Internet. In Westbrook J.H. & Fleischer, R.L. (Eds.) *Intermetallic Compounds: Principles and Practice* (Vol. 3, pp. 857-873). Chichester, UK: J. Wiley.
- Westbrook, J.H. & Grattidge, W. (1991) The Role of Metadata in the Design and Operation of a Materials Database. In Kaufman, J.G. & Glazman, J.S. (Eds.), *Computerization and Networking of Materials Databases*, STP 1106. Philadelphia: American Society for Testing and Materials.
- Westbrook, J.H. & Kaufman, J.G. (1996) Impediments to an Elusive Dream: Computer Access to Numeric Data for Engineering Materials. In Dubois, J-E. & Gershon, N. (Eds.) *Modeling Complex Data for Creating Information* (pp. 125). Berlin: CODATA/Springer.
- World Wide Web Consortium (n.d.)Homepage of the World Wide Web Consortium. Available from: <http://www.w3c.org/Consortium/>

Table 1. Directories

<p>Data Sources in China (http://sect.cnodata.ac.cn)</p>	<p>90 sites are listed, only a fraction of which are exclusively concentrated on materials</p>
<p>Edinburg Engineering Virtual Library EEVL (http://eevLic.hw.ac.uk)</p>	<p>the UK equivalent to EELS with links to >400 quality engineering sites on the Net</p>
<p>Gerry Lushington's Site (http://129.237.102.31/~msg/MGM/links/mats.html)</p>	<p>provides links to >50 sites, directories, and relevant downloadable programs</p>
<p>Google (www.directory.google.com)</p>	<p>a directory built by the Google search engine</p>
<p>Japanese Material Information Sites (http://inaba.nims.go.jp/netnavi-F0831.htm)</p>	<p>about 70 sites are listed, only a few of which are Japanese</p>
<p>STN (www.stn-international.de)</p>	<p>95 database producers and their websites are given, many of which relate to materials, but the collection is a mix of bibliographic and numeric databases</p>
<p>Swedish Universities Technical Libraries EELS (http://eels.lub.lu.se)</p>	<p>an amalgamation of websites and other information sources available through Swedish libraries</p>
<p>Virtual Library (http://vlib.org)</p>	<p>14 directories including several pertinent to materials, e.g. physics, ceramics, and chemical engineering</p>
<p>World Wide Web Virtual Library (http://www.vlib.org)</p>	<p>a distributed library located at many different sites around the world, built and maintained by volunteers who cover >100 individual subjects</p>
<p>Yahoo (www.Yahoo.com)</p>	<p>a humongous hierarchical index, created by humans to search the Web; hence, relative to the usual search engines it is more logical, less error-prone and more efficient</p>

Table 2a. Disciplinary Metasites

Chemistry

World Wide Web Hub for Chemistry (<http://einet.net/galaxy:Science/chem.html>)

Internet Chemistry Resources (<http://rpi.edu/dept/cheminfo/chemres.html>)

Chemistry Links (www.liv.ac.uk/Chemistry/Links/links.html)

Chemistry Web (<http://www.ss.ntu.edu.sg:8000/chemweb/>)

ChemCenter (www.ChemCenter.org) homepage of the American Chemical Society

Crystallography

Pauling File (www.PaulingFile.com)

Naval Research Laboratory (www.nrl.navy.mil/lattice/pearson.html)

Landolt-Börnstein (<http://link.springer.de/series/lb>)

Engineering

Engineering Resources Online (www.er-online.co.uk)

CRC Press (www.engnetbase.com) 145 online handbooks

Materials

Materials Science Resources on the Internet (<http://www.geocities.com/SiliconValley/5978/materials.html>) this site was originally developed by Cathy D. Stewart of National Steel and since augmented by Antonio Gorni of COSIPA-IME. It contains 13 pp. of listed sites.

The Virtual Materials Science Center (www-sci.lib.uci.edu)

MAP Data Library (www.msm.cam.ac.uk/map/data/data-index.html)

MaterSci (www.matersci.net)

MetalInfo (www.metalinfo.com) an online interactive portal called the “Atlas of World Metals”, which links the online search of more than 160,000 global metal engine and databases standards, more than 150,000 company profiles and thousands of dimensional tolerance standards

Composites Materials Handbook (www.mil17.org)

World Wide Web Virtual Library-Ceramics (<http://www.ikts.fhg.de/vl/ceramics.html>)

American Ceramic Society (www/acers.org/cic/propertiesdb/esp)

Minerals

Mineral Gallery (mineral.galleries.com/default.html)

Mineralogy Database (<http://webmineral.com>)

Physics

Physics Web (<http://physicsweb.org/Tiptop>)

WWW Virtual Library – Physics (www.w3.org/hypertext/DataSources/bySubject/Physics/Overview.html)

Technical University of Vienna (<http://tph.tuwein.ac.at/physics-services.html>)

Fachinformationszentrum (Karlsruhe) (www.fiz-karlsruhe.de)

Database for Atomic and Plasma Physics (<http://plasma-gate.weizmann.ac.il/DBtable.html>)

Table 2b. Institutional Metasites

<p>AMPTIAC (http://ListofDatabases.amptiac.iitri.org)</p> <p>Arizona State U. Library (www.asu/lib/noble/chem/prop-2htm)</p> <p>Center for Information and Numerical Data and Analysis (CINDAS) (http://CINDAS.www.ecn.purdue.edu/CINDAS)</p> <p>ELDATA (http://stn.permcti.ru/eldata/fk11.html)</p> <p>U. Illinois at Chicago (http://uic.edu/~mansoori/Thermodynamic.Data.and.Property_.html)</p> <p>International Atomic Energy Agency (www.iaea.or.at/database/dbdir/fulllist.htm)</p> <p>Martindale's Reference Desk (www.sci.lib.uci.edu)</p> <p>NIST Web Book (www.webbook.nist.gov), (www.nist.gov.srd)</p> <p>NRC (Canada) Industrial Materials Institute (www.imi.nrc.ca/umenglish.html)</p>	<p>DOD's Advanced Materials & Processes Technical Information Analysis Center includes its own information site, MatPro with 43 databases, about half of which are numeric and 4 of its own property databases (Al-Li alloys, intermetallics, austempered ductile iron, and silicon).</p> <p>an extensive site with reference to both chemical and materials data</p> <p>an integrated system of databases on physico-chemical (mainly thermo-physical and thermodynamic) properties of single or multi-component materials systems</p> <p>actually, much broader than thermodynamics; lists data sites, calculation programs, downloads, computer simulations, organizations involved with data compilation, and a bibliography of same</p> <p>a very broad information center including bibliographic and tutorial sites, glossaries, etc. in addition to numeric databases of materials properties, physics, chemistry and biochemistry</p>
---	--

Table 2c. Application Metasites

Hazardous Materials

<http://hazmat.dot.gov>
www.chemweb.com/databases/brchd
<http://ull.chemistry.uakron.edu/erd>

Materials Safety Data Sheets (MSDS)

www.mssl.ucl.ac.uk
www.msdssearch.com
www.ilpi.com/msds
www.msdsonline.com
<http://hazard.com/msds>
<http://physchem.ox.ac.uk/MSDS>
www.mdli.com

Metal Machining and Fabrication

www.mmf.com/metal/index/html

Micro-Electro-Mechanical Systems (MEMS)

www.memsnet.org/material
www.darpa.mil/MTO/MEMS
<http://memsindustrygroup.org>

Non-destructive Testing & Evaluation

www.dtic.dla.mil/iac/ntiac.ndelist.html

Nuclear Materials

Data-Free-Way <http://inaba.nims.go.jp/fujita.html>

Surface Science

www.uksaf.org/data.html
www.nist.gov/srd/surface.htm

Toxicology

<http://toxnet.nlm.nih.gov>
<http://see.msfc.gov/see/mp/database.html>
<http://www.cmdl.noaa.gov>

Welding

<http://vanbc.wimsey.com/robertsa/welding.html>

Table 2d. Topical Metasites for Basic Information

Fundamental Data

Web Elements www.webelements.com; general, physical, chemical, electronic, etc. properties of first 112 elements

Fundamental Physical Constants <http://physics.nist.gov/cuu/Constants/index.html>

Table of Nuclides <http://www.dne.bnl.gov/CoN/index.html>

The Periodic Table

University of Sheffield www.webelements.com/index.html

Chemicool at Massachusetts Institute of Technology www-tech.mit.edu/Chemicool/

Pictorial Periodic Table www.chemlabs.pc.maricopa.edu/periodic/periodic.html

Materials World Web www.geocities.com/materialsworldweb/Periodic_T.html

Yinon Bentor's Site www.chemicalelements.com

Phase Diagrams

Georgia Tech www.cyberbuzz.gatech.edu/asm-tms/phase_diagrams data, tables, diagrams, evaluations, and references for many but not all binaries

Materials Science International (Stuttgart) www.msiwp.com

GTT Technologies at Herzogenrath, Germany <http://gttserv.lth.rwth.aachen.de>
1000s of the systems included in ASM's binary and ternary collections and from American Ceramic Society's 13,000 systems. Many of these are sold as sub-collections on CD-ROM or single systems are offered online for a fee.

STGE www.met.kth.se/pd/calc This cooperative European group summarizes their work on calculated diagrams.

Standards

IHS Engineering Products www.ihs.com

Contacts for purchase of standards, but no direct access

www.metalinfo.com

www.principalmetals.com

www.grantadesign.com

www.iso.ch (International Standards Organization)

www.nssn.org (ANSI)

www.astm.org/standards (ASTM)

Table 2e. Some Unusual Specific Sites

<p>Acoustic Material Property Tables (www.ultrasonic.com/tables/index.htm)</p> <p>Biomaterials Properties (www.lib.umich.edu.dentlib/Dental_tables/toc.html)</p> <p>Building Stone (www.wishbone.com)</p> <p>Center for Atomic Scale Materials Physics, Technical University of Denmark (www.fysik.dtu.dk)</p> <p>Jahm Software (www.jahm.com)</p> <p>Physical Properties of Soils (http://homepages.which.net/~fred.moor/soil/links/10101.htm)</p> <p>Smart Materials (www.sciam.com/explorations/050596explorations.html)</p> <p>Spacecraft Structural Engineering (FRAMES-2) (http://esapub.esrin.eas.it/pff/pffv6nl/env6nl.htm)</p>	<p>45 properties of dental restorative materials together with 244 source references</p> <p>the varieties and properties of natural building stone, e.g. granite, marble,....</p> <p>mostly concentrates on: growth of materials, nanostructures, interfaces, chemical properties of surfaces</p> <p>A database of temperature-dependent elastic and thermal properties.</p>
---	--