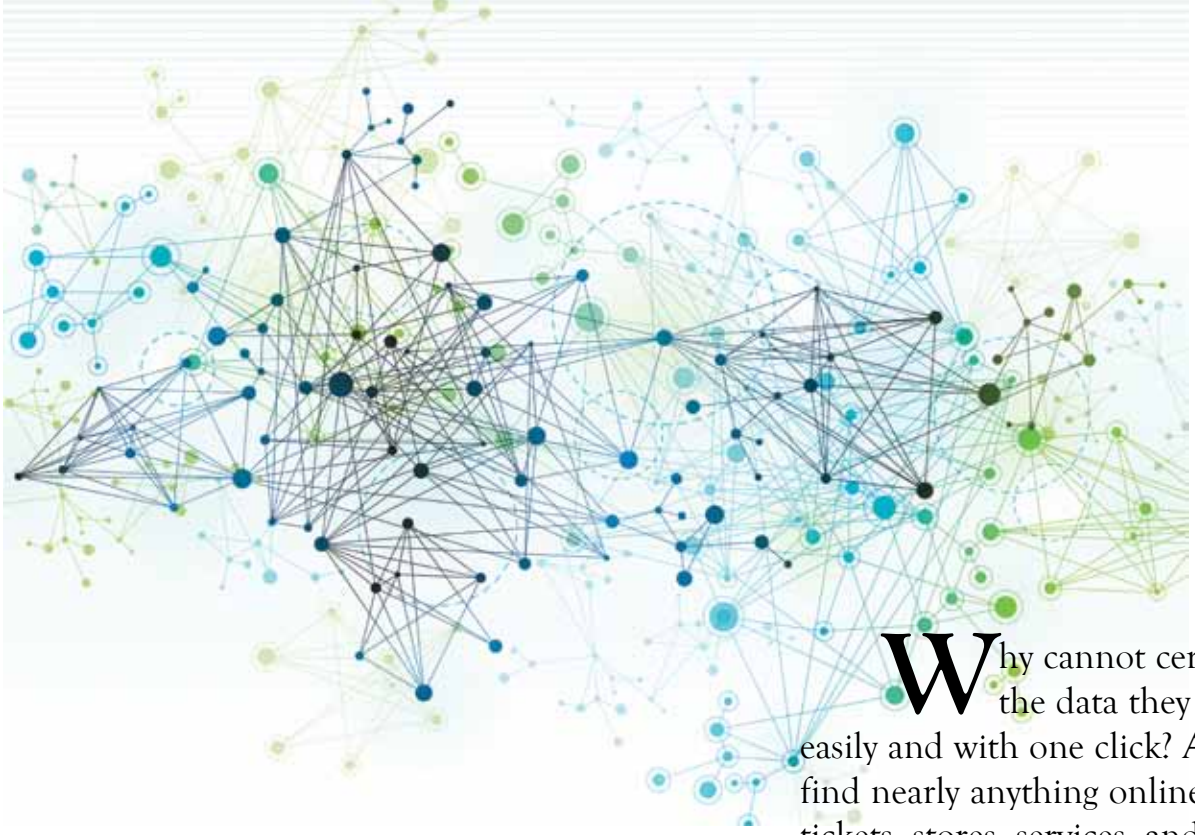

Current availability of ceramic property data and future opportunities

By Steve Freiman and John Rumble

It is time for the ceramics community to work toward establishing a comprehensive ceramic property database that is easily assessable through a single entry point

Why cannot ceramists get all the data they need online—easily and with one click? After all, we can find nearly anything online—hotels, airline tickets, stores, services, and everything else. Why is it so difficult to find high-quality ceramic property data online?

To help answer these and similar questions, we recently completed a study for the Department of Defense on the availability of and access to ceramic data and what could be done to improve the situation. Our work focused on three critical questions.

- What ceramic property data are actually available online today?
- What ceramic property data do people want and why?
- What can be done to improve the quality and availability of ceramic data?

We found that many datasets are available online, but are distributed in a difficult-to-navigate maze of unconnected databases, in many different formats, using nonstandard terminology. The situation is far from the single access point users want, and the quality of available data is difficult to judge.

What can be done? It is time for the ceramics community to overcome barriers resulting from proprietary interests, high start-up costs, and uncoordinated data efforts and work together to build a modern ceramic property data system that will aid discovery of new materials and promote selection of advanced ceramics for new products and applications. We have the opportunity to make progress, as we outline below.

Background

The ability to generate, store, manage, and reuse large amounts of data is driving new modes of scientific research, including data mining, modeling and simulation, and knowledge discovery. The globalization of research means that significant science and technology datasets generated in one country are useful and needed by researchers

worldwide. Even though most material property data are generated by "small" science (that is, by individual researchers or small research groups), in aggregate, the entire body of materials research results constitutes a large dataset that is increasingly important to state-of-the-art research. For example, the Materials Genome Initiative in the US, whose goal is to expedite the transition from new materials development to incorporation in a final product, demands better access to accurate property data.

We can find hotels, air tickets, stores, and everything else online. Why is finding high-quality ceramic property data so difficult?

Unfortunately, access to materials property data today is haphazard. There is no single entry point. Datasets that are found using existing search engines are of unknown quality and provenance. In fact, no individual data resource is comprehensive with respect to properties or materials.

Our year-long study supported by DOD focused on the electronic availability of ceramic property data as an exemplar of the larger realm of materials data. During the 20 years since the Internet and the World Wide Web revolutionized access to data and information, numerous online data resources covering virtually all ceramic materials and properties have been created. Because these data resources are maintained by diverse, independent organizations, locating and gaining access to specific datasets remains a challenge, despite the power of modern search engines to help discover them.

As part of this study, we performed an intensive search for web sites containing ceramic property data. The goal was to locate as many resources as possible and characterize each of them with respect to content, availability, fee structure, and coverage. Our aim was to create a database of ceramic property electronic databases for use by organizations as a basis for developing easier, more cohesive access to multiple data resources for users. Although we focused primarily on electronic resources, we identified several important print sources and include them in this report.

Status quo: Ceramic property data available online today

What ceramic property databases actually exist? First, let us define ceramics to mean any inorganic nonmetal, including zeolites and minerals. The next question is, which databases are important? While databases containing citations, abstracts, or full text articles on ceramics are found easily, databases containing numerical data on ceramic properties are scarce. We looked for data for various forms of ceramics (i.e., single crystal, polycrystalline, glasses, fibers, films, composites, and coatings), and included structural, thermal, mechanical, and optical properties.

Because no one single access point (portal) or directory for ceramic property data exists, we used multiple search engines and multiple languages to search the entire web thoroughly, often using professional searchers. No wonder the average scientist or engineer looking for ceramic property data gets frustrated with the difficulty of finding what the need!


(Credit: ACerS)

John Rumble leads a discussion on ceramic property data at a DOD-sponsored workshop, June 2012.

A substantial quantity of ceramic property data exists in journal articles and has not been extracted and compiled into databases, whether print or electronic. Also, many national laboratories, universities, and other research institutions have collections of ceramic property data that are not publicly available.

In our research we identified more than 100 possible ceramic property data resources, but we exclude those without property data (and there were many) from our list of databases. The complete annotated list of ceramics data resources is available at www.ceramics.org. (See condensed list, page 38-39.)

We observed some general trends regarding the availability of ceramics property data.

- ***Although considerable amounts of ceramics property data are available, no single resource is comprehensive.*** Most resources concentrate on one or a few properties. The few databases that attempted to be comprehensive were not up-to-date or covered only portions of the world's research literature. None clearly stated what procedures were used to locate data nor the selection criteria for data in the database. An individual user most likely would have consult several resources to find the needed data.
- ***Many data resources are no longer being updated.*** Many important resources are not being updated. Rarely does a resource clearly indicate the years of coverage. As a result, property data for newer ceramic materials are difficult to find, delaying adoption of these newer ceramics.
- ***Data quality indicators are lacking for most data resources.*** Even when data are located, their quality and provenance are rarely indicated. Long-term data evaluation programs, such as the ACerS-NIST Phase Diagram for Ceramists Program and the various crystallographic data centers, are exceptions rather than the rule. Quality verification is necessary before using property data found in most databases for critical applications. The lack of quality indicators for fundamental data, such as elastic constants, will be a barrier to using results from

modeling and simulation in the future.

• ***In aggregate, many types of properties are not adequately covered in databases, including some fundamental ceramic properties, even if they have been measured and reported in the literature.*** Data for many properties, including routine standard test results, are not in these databases. When included, the accompanying metadata—for example, compositional information, test procedure, and statistical analysis—are not given.

• ***Performance data are incomplete, and historical coverage of these properties is lacking.*** Incomplete coverage is especially the situation for performance properties. Many of these data, even if reported in the literature, are buried in government and laboratory reports receiving little circulation. Many sets of ceramic performance data were generated for specialized energy and defense programs, especially for more extreme conditions. These data sets are rarely included

• ***No single point of access exists.*** The hunt for ceramic property data requires multiple searches through multiple data resources to locate all desired data. There is not even a comprehensive directory of databases available, much less an index of the all materials and properties. Even when an individual database is accessed, determining its contents can be difficult and time consuming. Unlike many other disciplines such as astronomy and its International Virtual Observatory (www.ivoa.net), no progress has been made on creating a one-stop access point (data portal) for ceramic property data.

• ***Differing fee structures for subscription-based resources.*** Vendors of subscription-based ceramic property databases present customers with a variety of fee structures, user agreements, and software or hardware requirements. These arrangements can present significant barriers, including justifying subscriptions to managers, and in some cases, employer-imposed restrictions on accessing outside web services.

These issues represent major challenges.

(Credit: ACerS)

Workshop participants discuss their ceramic property data needs and challenges.

From the data provider perspective, some challenges may reduce the number of customers. However, without revenue from subscriptions, fee-based models would probably cease to exist. From the data seeker perspective, these challenges reduce the amount of available data. From the ceramic community perspective, these challenges represent barriers to advancing the use of ceramics in industry.

What ceramic property data do people want and why?

Answering this question is crucial for designing future access to ceramic property data. After all, there are many types of ceramics with various properties, and data needs vary accordingly. For example, development engineers may be satisfied with lower-quality data for preliminary design work, whereas others may need high-quality, verified data to formulate a detailed processing specification for a critical component of an airplane made of advanced ceramics.

The authors brought together experts to evaluate whether the needs of industry, government laboratories, and academia for electronic access to ceramic property data are being met, and if not, what actions are needed to meet those needs. The "Workshop on E-Ceramics: Prospects and Challenges for Improved Access to Ceramics Property Data," was held in the Virginia Tech Research Center in Arlington, Va., June 4–5, 2012. We opened the meeting by presenting the results of our survey of ceramic data resources. We asked attendees to identify data needs from their sectors (industry, government, academia).

Speakers agreed that their needs for ceramic-related property data covered the entire spectrum of ceramic materials and included

• Composition, structure, and phase information;

• Processing and post-processing data;

• Fundamental properties needed for modeling, such as finite-element analysis;

• Performance properties;

• Specialized properties, such as electrical, optical, and piezoelectric; and

• Failure information.

Major recommendations made by the participants include,

• There should be open access to the database of ceramic property databases compiled under this study.

• There should be a concerted effort to build a high-quality database of fundamental properties of single crystals to support atomistic scale modeling. Elastic and electrical constants and similar data should be included to support finite-element analysis and other modeling techniques.

• Work should be restarted on establishing metadata guidelines for ceramic property data, perhaps under the auspices of ASTM C28 on Advanced Ceramics.

• The ceramics community should be surveyed regarding the need for new data evaluation projects for ceramic property data, including performance data. Possibile projects include updating the NIST Ceramics WebBook or creating electronic access to print data compilations.

• The feasibility of establishing a ceramics data portal to provide a single point of access to as many ceramics data resources as possible should be explored. This may be an appropriate activity for an organization such as the American Ceramic Society.

• International Traffic in Arms Regulations (ITAR) should be reviewed, in particular, restrictions that, in some cases, limit sharing of data on advanced materials, especially ceramic matrix composites.

• Journals should provide access to article data tables and even to the raw data on which tables are based—perhaps, for example, with data repositories built

and maintained by the journals themselves, by professional societies, or by other organizations.

• Continuing material property data workshops and conferences should be conducted that foster the exchange of knowledge and promote progress in this area.

The consensus opinion expressed by attendees at workshop and by others in discussions we had during our study, is that user access to ceramic property data falls short of the need. How best can interested parties—industrial product designers, component manufacturers, and government agencies—meet those needs? We must recognize that ceramic property data are important enough that companies and institutions have historically been willing to pay for access to data in handbooks, commercial databases, individual databases, and research programs. The economic value of ceramic property data is well established, and fee-based services are accepted.

At the same time, ceramic property data are usually just one input into the complicated, nonlinear development of commercial products or materials. Often, property data are critical in the early stages of product conceptualization and design, but the final product reaches the market several years later. The conundrum is that the value of property data is recognized, but its importance in the long-term economics of a final product is vastly underestimated

In addition, the properties of engineering materials, especially ceramics, varies considerably with small compositional, processing, and manufacturing changes. Many ceramics, for example, are individually tailored by their manufacturers to meet specific product needs. As a result, general ceramic property data help guide general materials selection, but additional data or new measurements are often involved before making a final selection.

Improving quality and availability of ceramic property data

The responsibility for meeting the needs of a general user of ceramic property data is not clear cut. Professional societies, which collectively provide much of the materials property data in the US, struggle to find a sustainable business model for providing a one-stop service for ceramic data. Government agencies, especially in the areas of defense, energy, and security, have limited mandates. Large commercial data providers see limited market potential for the ceramics subset of materials. Although small commercial data providers claim to provide comprehensive coverage, in fact, their data products are outdated, incomplete, or both. Ceramic manufacturers, understandably, limit their scope to only their materials.

How then can the ceramics data user community coalesce and provide a coherent argument for meeting their needs? Based on our observations of activities in other scientific and technical disciplines, several potential approaches can be identified.

We begin by defining our view of the ideal solution for accessing ceramic property data, and that is an online system that provides single-point access to all ceramic property data resources. We envision it having these characteristics:

1. Single-point-of-entry portal exists to all ceramic property data resources;
2. Users subscribe to one service only;
3. Portal lists all ceramic materials for which there is data and describes the property data available;
4. Directory lists all known synonyms for materials and properties;
5. System has a variety of display options and analytical tools;
6. All data should has quality indicators;
7. Primary interface is adaptable by the user and supports various languages; and
8. Mobile device applications are supported.

Today's ceramic property data system ignores the benefits of the modern information age.

In contrast, today we have a diffuse and uncoordinated ceramic property data system with the user having to contract separately with each data resource and through multiple interfaces. In practical terms, Google, Yahoo, or other search engines often act as the point-of-entry. This is unsatisfactory from many perspectives, not the least of which is the lack of selectivity among search results. Finding, accessing or linking to each identified data resource is the responsibility of each individual user or institution. Further, such a system does not provide detailed information about the contents of each data resource, and the utility and coverage of a resource often cannot be determined without considerable effort. In some cases, a database's contents cannot be vetted until license contracts are in place.

Today's ceramic data system does not meet user needs, acts as a barrier to adopting ceramic materials, and fails to maximize the tools offered by the modern information age. There are challenges to creating the ideal solution.

The cost of building and maintaining a monolithic data system is significant, even with all the advances made in information technology and web technology during the past 20 years.

• No standards exist for describing ceramic materials or ceramic property data.

• An effort to integrate data from the more than 50 ceramic property data resources identified in this report would be daunting.

• Many of the data resources are proprietary and are designed to be revenue sources for their builders or providers. They have little economic incentive to cooperate with a monolithic system.

Yet, a robust ceramic property data system that inherently meets user needs is possible. In fact, there could be multiple points-of-entry via multiple systems, depending on the marketplace. Under this model, each system would be similar in many respects and would likely include the following characteristics.

1. A single access point—or data portal—would be operated by a system provider.
2. Users would have one contract with the system provider.
3. The system provider would have contracts with as many data resources as possible, such that a user wanting to use a resource would need only to invoke the user–system provider contract.
4. Over time, the system provider

would create detailed directories of the content of all data resources to make it easy for users to locate needed data.

5. The system provider initially would provide a simple, easy-to-execute link to individual data resources.

6. Over time, the system provider would develop standard displays, tools, and cross-data resource searching capability.

7. Access to data resources through a quality system provider would provide some level of data quality that would increase over time as users return to the system.

The market for single point access, modern ceramic property data system is there, waiting to be exploited!

How do we get there?

With more than 50 data resources containing ceramic property data available today, coverage in terms of materials and properties likely is sufficient to attract a critical number of users to generate the revenue necessary for a sustainable system—if all available data are easily accessible. The market for single-point access, modern ceramics data system is there, waiting to be exploited!

To help provide momentum, the ceramics community can take the following important steps.

- The directory of ceramics databases produced by this study is freely available to interested parties and is published on the ACerS website at www.ceramics.org/knowledge-center. We encourage readers to identify other ceramic property data resources that should be added and send them to ACerS at customerservice@ceramics.org.
- Federal agencies should make their substantial, publicly available collections of ceramic property data developed in support of the programs more easily discoverable.
- A concerted effort is needed to build a high-quality database of fundamental properties of single crystals to support atomistic scale modeling, including elastic and electrical constants. The database should be capable of supporting FEM and other modeling techniques.
- Work should restart on establishing metadata guidelines for ceramic property data. This work could be done under the auspices of ASTM C28 on Advanced Ceramics.
- Journals should provide access to data tables and even the raw data behind tables in their articles through data repositories that could be built and maintained by the journals themselves, by professional societies, or by other organizations, similar to the data repositories operated by crystallographic data centers, such as the FIZ/NIST Inorganic Crystal Structure Database.

The time has come for the ceramics community to join the 21st century and be able to access all ceramic property data easily and through a single entry point. Users, want it; the ceramics industry needs it; and the tools are available. Let's make it happen.

Acknowledgements

The authors acknowledge support from the Department of Defense to perform most of this work. We thank June Crowe and Diane Rumble for their help locating ceramic property data resources.

About the authors

Steve Freiman is principal with Freiman Consulting, Potomac, Md., and John Rumble is president of R&R Data Services, Gaithersburg, Md. Contact: Steve Freiman at steve.freiman@comcast.net; John Rumble at jumbleusa@earthlink.net ■

Selected ceramic property data resources.

Visit www.ceramics.org/knowledge-center to view the workshop report and a complete listing of ceramic property data resources.

Table 1 Comprehensive and general ceramics databases—government and universities

Builder or maintainer	Name	URL
National Institute of Standards and Technology	Ceramic WebBook	http://www.ceramics.nist.gov/webbook/evaluate.htm
National Institute of Advanced Industrial Science and Technology (Japan)	Network Database System for Thermophysical Property Data	http://riodb.ibase.aist.go.jp/TPDB
	Optical Properties of Ceramics and Ceramics Thin Films	http://riodb.ibase.aist.go.jp/opcc
	CCDB Glaze Database	http://riodb.ibase.aist.go.jp/ccdb
	RASMIM (Raman Spectra Database of Minerals and Inorganic Materials)	http://riodb.ibase.aist.go.jp/rasmin
	Mat Navi, NIMS Materials Database	http://mits.nims.go.jp
Korean Institute of Ceramics Engineering and Technology (South Korea)	Mat Bank	http://matbank.org/
Japan Aerospace Exploration Agency (JAXA) (Japan)	Materials Database	http://matdb1n.tksc.jaxa.jp/MaterialEvaluation/
National Physical Laboratory (U.K.)	Kaye & Laby Tables of Physical and Chemical Constants	http://kayelaby.npl.co.uk/
University of Caen Basse-Normandie (France)	Materials Properties Open Database	http://www.materialproperties.org/data/
Bundesanstalt für Materialforschung und –prüfung (Germany)	Tribocollect	http://www.bam.de/php/tricot/tricot_voll.php
Massachusetts Institute of Technology	Materials Project	http://materialsproject.org/
National Aeronautics and Space Administration Ames Research Center	Thermal Protection Systems Expert and Material Properties Database (TPSX)	http://tpsx.arc.nasa.gov/
Matbase Group (Netherlands)	MATBASE	http://matbase.com
University of Dayton Research Institute	Ceramics Summary and Design Data Files (Compendium)	http://www.udri.udayton.edu/EnergyTechnologiesAndMaterials/AdvancedHighTemperatureMaterials/Pages/CeramicsSummaryandDesignDataFiles.aspx

These online databases, built and maintained by government agencies and research institutes and universities, contain data on ceramic materials for multiple properties under a variety of conditions. In the aggregate, they provide substantial coverage of available ceramic property data, however, individual databases have limited coverage.

Table 2 Comprehensive and general ceramics databases—commercial database providers

Builder or Maintainer	Name	URL
MatWeb LLC	MatWeb	http://www.matweb.com
CINDAS LLC	Thermophysical Properties of Materials Database (TMPD)	http://cindasdata.com/
	Microelectronic Packing Materials Database (MPMD)	http://cindasdata.com/
Granta Material Intelligence (UK)	Granta Data Series	http://grantadesign.com/products/data
Matereality LLC	Matereality Global Data Center	http://www.matereality.com/
JAHM Software Inc.	JAHM Software	http://www.jahm.com/index.html
Material ConneXion	Material ConneXion Online Materials Database	http://www.materialconnecxion.com/
ProQuest, Cambridge Information Services	ProQquest Deep Indexing: Materials Science	http://www.csa.com
Makeitfrom	Materials Properties Database	http://www.makeitfrom.com/
eFunda Inc.	efunda	http://www.efunda.com/materials/piezo/material_data/matdata_index.cfm

These online databases, built and maintained by commercial database providers, contain data on ceramic materials for multiple properties under a variety of conditions. In the aggregate, they provide substantial coverage of available ceramic property data, however, individual databases have limited coverage.

Table 3 Ceramic materials producers databases (selected examples)

Builder or Maintainer	URL
Dynallox Alumina Ceramics	http://dynacer.com/PDF/dynalloxproperties.pdf
Morgan Technical Ceramics	http://www.mtcmaterialscomparator.com/
Boston Piezo-Optics Inc.	http://bostonpiezooptics.com
Coorstek	http://www.coorstek.com/resource-library/library/8510-1042_ceramic_material_properties.pdf
Du-Co Ceramics	http://du-co.com/properties
Accuratus	http://accuratus.com/
Ceradyne	http://www.ceradyne.com/
Morgan Technical Ceramics—Properties of Piezoelectricity Ceramics	http://traktoria.org/files/sonar/piezoceramics/morgan/properties_of_piezoelectric_ceramics_(pzt-4_pzt-5a_pzt-5h_pzt-8).pdf
Materials Science and Engineering Department, State University of New York at Stony Brook. This site provides a list of companies specializing in ceramics. Each company likely has material property data sheets on their website.	http://www.matscieng.sunysb.edu/other4.html#manufact

Many company websites now provide product description data on the composition and properties of their ceramic products. In most instances the data are limited to their own products and have not been published in the journal literature. The State University of New York at Stony Brook maintains a list of ceramic producers and is a good resource for locating product data sheets.

Table 4. Glass databases

Builder or Maintainer	Name	URL
Scimatics Information System	SciGlass Property	http://www.sciglass.info/
New Glass Forum (Japan)	INTERGLAD	http://www.newglass.jp/interglad_n/gaiyo/info_e.html

Table 5 Ceramic phase equilibria and crystal structure databases

Builder or Maintainer	Name	URL
National Institute of Standards and Technology and The American Ceramic Society	Phase Equilibria Diagrams	http://ceramics.org/publications-and-resources/ phase-equilibria-diagrams
FIZ Karlsruhe (Germany) and National Institute of Standards and Technology (Germany)	Inorganic Crystal Structural Database (ICSD)	http://fiz-karlsruhe.de/icsd/html
Basque University (Spain)	Bilbao Incommensurate Structures Database	http://158.227.21.14/instrdb/
Mineralogical Society of America and Mineralogical Society of Canada (Canada)	The American Mineralogist Crystal Structure Database	http://www.minsocam.org/msa/crystal_database.html
Institute of Experimental Mineralogy, Russian Academy of Sciences (Russia)	WWW-MINCRYST	http://database.iem.ac.ru/mincryst/index.php
Structure Commission, International Zeolite Association	Database of Zeolite Structures	http://www.iza-structure.org/databases/

Phase equilibria diagrams and crystallographic structure are fundamental properties of ceramic materials and are the subject of several databases, all of which heavily emphasize evaluating the quality of data included in this table.

Table 6 Other ceramics-related databases

Organization	Location	URL
The American Ceramic Society	Westerville, Ohio	http://ceramics.org
ASM International	Materials Park, Ohio	http://www.asminternational.org/
Mindat.org	Mindat, Coulsdon, Surrey, England	http://mindat.org
Materials Digital Library Pathway (MatDL)	Kent State University, Kent, Ohio	http://matdl.org
Advanced Materials, Manufacturing, and Testing Information Analysis Center (AMMTIAC)	Alion Science, Rome, N.Y.	http://ammtiac.alionscience.com

Several professional societies and information organizations provide or link to data resources related to ceramics.

Table 7 Ceramics-related data publications (print)

Publication	Editor	Publisher
CRC Materials Science and Engineering Handbook	Edited by J.F. Shackelford, W. Alexander, and J.S. Park	CRC Press, Boca Raton, Fla. (1994).
Thermal and Other Properties of Refractories, Technical Report Program No. R056	Los Alamos National Laboratory	Los Alamos Scientific Laboratory, Los Alamos, N.M (1973)
Single Crystal Elastic Constants and Calculated Aggregate Properties: A Handbook, 2nd Edition	Edited by G. Simmons and H. Wang	MIT Press, Cambridge, Mass. (1971)
Elastic Moduli Data for Polycrystalline Oxide Ceramics	Edited by R.G. Munro	NIST Internal Report 6853, Gaithersburg, Md. (2002)
Handbook of Optical Constants of Solids II	Edited by E.D. Palik	Academic Press (1991)
Data Evaluation Theory and Practice for Materials Properties: NIST Recommended Practice Guide 960-11	Edited by R.G. Munro	NIST, Gaithersburg, Md. (2003)

Many print-only compilations of critically evaluated data are still valid decades after their publication.