E-Ceramics 2012

The Availability, Quality, and Location of Ceramic Property Data

A Study Performed by

Information International Associates, Inc.

Oak Ridge, Tennessee

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Nov 20, 2012

Foreword

This report reviews the present day status of the availability, quality, and location of ceramic property data as performed under contract number N00167-11-P-0533 from the Department of Defense. The purpose of the study was both to assess the current availability of ceramics property data and to identify potential new activities by the government and the private sector to improve the accessibility and quality of materials data. The area of ceramic property data was selected as an exemplar to highlight not only present-day status, but also next steps that could be taken by various parties.

The work consisted of three major parts: identifying data resources now available, a workshop to define emerging needs for materials data access in the future, and a review of data activities in Asia, (Japan, Korea, and China). Based on the results of these efforts, a variety of business approaches were identified including roles for different stakeholders.

A set of recommendations is included based on the investigators' personal knowledge and conclusions. No endorsement by the Department of Defense or any other U.S. Government agency is implied.

Comments and questions should be sent to the first two investigators listed below.

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Section1. Introduction, Conclusions, and Recommendations

1.1 Introduction

The availability of materials data is a critical component of Department of Defense (DoD) strategy to maintain world leadership in science and technology in support of its missions for the military, national security, and others, while adhering to current fiscal constraints. As DoD and its contractors design, build, and operate next-generation hardware systems, taking advantage of new and improved materials is an important key to the success of those systems.

The importance of access to high quality scientific and technical (S&T) data has become increasingly apparent in this age of data-intensive science. The ability to generate, store, manage, and reuse large amounts of data has driven new modes of scientific research, including data mining, modeling and simulation, and knowledge discovery. In addition, the globalization of research means that significant S&T data sets generated outside the United States should be available to U.S. researchers. Even though most materials 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 data set that is increasingly important to state-of-the-art research in the future.

Unfortunately, access to materials property data today is haphazard. There is no single entry point, and data sets that are found using today's search engines are of unknown quality and provenance. In fact, no individual data resource is comprehensive with respect to properties or materials. Therefore, DoD has contracted with Information International Associates, Inc. (IIa) and its subcontractors—R&R Data Services, Freiman Consulting, and the Asian Technology Information Program—to assess current availability, accessibility, and quality of materials property data. This study focuses on ceramic property data as an exemplar of materials data to allow for full understanding of the scope of problems within a manageable case study.

The work comprised several subtasks to provide information, guidance, and insight for DoD's investments and decision-making regarding state-of-the-art access to data and information on ceramic materials and their known properties. The hope is to create one or more self-sustaining, single-access points of entry (data portals) to many or all ceramic data resources that are open to the global community. The initial investment and study objective has been to assess the state of the data in the community (inside and outside the United States) and to develop options for a business plan to determine how to provide state-of-the-art access to ceramic property data. The work consisted of three tasks:

Task 1a. Develop a report on the present-day availability of ceramic property data from open source (digital and print), government-owned, and restricted databases, reports, literature, publications, and unpublished sources, including detailed information of Chinese and Japanese activities in the area of ceramic property data. Detailed results are given in Section 2 and

Appendix B (for present-day availability of data) and Section 4 (for activities in China, Japan, and Korea, which was added after the study started as an additional reference point).

Task 1b. Determine options to develop models for web-based access to ceramic property data, as well as potential business models for such access. Detailed results are given in Section 5.

Task 2. Hold a ceramics informatics workshop, to include leaders in the industry and interested potential users that would assess user needs for ceramic property data. Detailed results are given in Section 3 and Appendix A.

From this work, several general conclusions and recommendations are made (Section 1.2), along with DoD-specific conclusions and recommendations (Section 1.3).

1.2 Overall Conclusions and Recommendations

U.S. leadership in materials research is critical for reaching our national defense, economic, and quality of life goals. Innovation and advances in materials today require access to materials data, regardless of where those data are generated or made available. For several decades, the United States was the world's leader in materials data activities through aggressive programs conducted by government agencies, professional societies, private data companies, industrial materials producers, and standards development organizations. However, our review of these activities throughout the world, especially in Asia, reveals that the United States is losing leadership in the area of ceramics (and likely all materials) property data.

To this end, we provide the following conclusions and associated recommendations.

Conclusion #1 – Limited Access to Data

Many ceramics data resources are available, developed and disseminated by diverse organizations. Full utilization of these resources is a challenge because of the following:

- Lack of a single point of access
- Proprietary data whose access is controlled for commercial, national security, or competitive reasons
- No comprehensive directory of resources, their content, or access methods
- No standardized content, especially in terms of the description of ceramic materials and their properties
- Few if any links to tools using the data
- Cost of accessing many of the available sites

Recommendations

- *Recommendations 1A.* The directory of ceramics databases produced by this study should be made freely available to interested parties, who in turn should be encouraged to develop access portals that take advantage of modern web and mobile application technology. As specified in the work statement, an article in

the ceramics press will be prepared that will include information for obtaining an electronic copy of the directory.

- *Recommendation 1B.* Federal agencies and private sector organizations should develop new or enhanced existing partnerships to take advantage of new information and web technologies such as the web, data portals, and data science to provide next generation access to materials data resources.

Conclusion #2 – Challenges to U.S. Leadership in Ceramics and Materials Data

- ***The U.S. leadership in ceramics, as well as other materials data in general, is being challenged*** and will require renewed commitment from government agencies, professional organizations, and U.S.-based information companies to maintain the U.S. leadership needed to support advanced materials development, next generation manufacturing, and exploitation of new technologies such as nanotechnology, bio-medical materials, and advanced performance products, including aircraft, automobile, and energy generation.

Recommendations

- *Recommendation 2A.* The United States should reaffirm its leading role in sharing knowledge about materials data and database activities and should also develop an international materials data conference series similar to those sponsored by ASTM International in the 1980s and 1990s. A first step might be to gain full partnership with the Asian Materials Database Symposium Series, perhaps by working to transform it to an Asian-Pacific Materials Database Symposium Series.
- *Recommendation 2B.* U.S. government agencies and professional materials organizations should develop a new *community of interest* to foster development and improvement of ceramics and materials data resources in the United States, including standards, data quality, and knowledge sharing.
- *Recommendation 2C.* Large-scale materials research programs such as the Materials Genome Initiative and the National Nanotechnology Initiative should directly fund materials data activities as an integral part of their research agenda.

Conclusion #3 – Goals for U.S. Leadership

- ***The growing importance of materials data in terms of U.S. leadership in materials research and engineering*** is a consequence resulting from many decades of investment in the information revolution. Whereas 30 years ago the United States had clear international leadership in materials data activities, the rest of the world, especially Asia, is catching and surpassing us. Our national goals in science, engineering, and manufacturing, however, require us to have the greatest possible capability for preserving, evaluating, and disseminating materials data.

Recommendation

- *Recommendation 3A.* Within a year, one or more federal agencies should sponsor an independent, in-depth review of U.S. materials data center activities, with special emphasis on examining the following:
  - The health of existing materials data activities within DoD, the National Institute of Standards and Technology (NIST), the National Science Foundation (NSF), and other agencies, including prospects for long-term financial support and integration within federal materials research programs
  - The status and future prospects of materials data programs supported by U.S. professional societies and independent data organizations and companies
  - Priorities for new materials data activities, especially to support materials advances in the next two decades, such as those required for computational materials science, critical materials substitution, and revolutionary materials advances as generated by technologies, to include nanotechnology, high temperature superconductors, and advanced composites
  - The need for next-generation materials data repositories and data sharing standards

Section 2. Task 1a.1 Available Ceramic Property Data

2.1 Introduction

In the twenty years since the internet and the World Wide Web have revolutionized access to data and information, the world-wide ceramics community has created numerous online data resources covering virtually all ceramics materials and properties. Because these data resources have been created and maintained by diverse, independent organizations, locating and gaining access to a specific piece of needed data remains a challenge, even with the existence of modern search engines.

As part of this study, we performed an intensive search for ceramics data resources. The goal was not only to locate as many resources as possible, but also to characterize them with respect to content, availability, fee structure, and coverage. Our ultimate aim was to create a database of ceramic property databases that could be used by organizations as the basis for developing easier, more cohesive access to multiple data resources for users. A second aim was to understand business models used by the individual data resources in order to build recommendations of a new business model for providing single point access (a data portal) to multiple resources (see Section 4). The results of our searches follow.

2.2 Available Ceramic Property Data

The primary objective for this effort was to assess the existence of ceramic property data, focusing on those data available electronically. In this context, we define the term *ceramics* to mean any inorganic non-metal, including zeolites and minerals. While databases containing citations, abstracts, or full text information on this topic are easily found, databases containing data on ceramic properties are scarcer. There is no one single portal for such data, and ceramic property data is part of the larger materials sciences subject area which covers chemistry and engineering.

Although our focus for this effort was on electronic sources, we did examine some known print ceramic property data sources, such as those published by CRC Press, Knovel, and ASM International. We also discovered a substantial quantity of ceramic property data in journal articles that does not exist in a database. As part of our initial strategy, we gathered some background information on the topic to clarify more specifically the needed ceramic property data for the effort. We narrowed down the data forms and the types of property data needed, and then we developed a template to use in reporting the information found. Ceramic data forms/materials could include the various forms (i.e., single crystal, polycrystalline, glasses, fibers, films, composites, and coatings). Data of interest included structural, thermal, mechanical, and optical properties. Our ability to locate foreign language data resources enabled us to find many non-English data sources of ceramic property data.

The primary search for ceramic property data was performed by experienced open-source search specialists at IIa. IIa has over 25 years' experience in searching for scientific, technical, engineering, and medical information for DoD and other government agencies.

Our search strategy was to explore the known sources, such as those at NIST, the American Ceramic Society, publishers, e.g., John Wiley, Springer, and others. After exhausting the known sites, we looked at academic institutions that had strong programs in material sciences such as those at the California Institute of Technology, the Massachusetts Institute of Technology, the Georgia Institute of Technology, Iowa State University, as well as others. We utilized the library subject guides on material sciences from these institutions to discover more sources.

We also searched for ceramic property data at the Department of Energy (DOE) laboratories. At DOE's Office of Scientific and Technical Information (OSTI), we had some success in locating foreign sources using worldwidescience.org, DOE's global gateway portal that connects scientific databases and portals from over seventy-five countries and international organizations. We also used Scirus.com, a comprehensive, science-specific engine that searches over 460 million science webs. The search strategy is depicted in Figure 1. In addition to the free internet sites, we also identified commercial databases such as Knovel, Chemical Abstracts Service, ASM International, and commercial suppliers that have databases of ceramic property data.

In the course of searching for foreign ceramic data sources, we discovered that many foreign countries defer to the data from NIST. As mentioned earlier, OSTI's worldwidescience.org

portal was very useful in discovering foreign sites for ceramic data. The CODATA register of materials database managers was also useful in discovering foreign sources of ceramic property data.

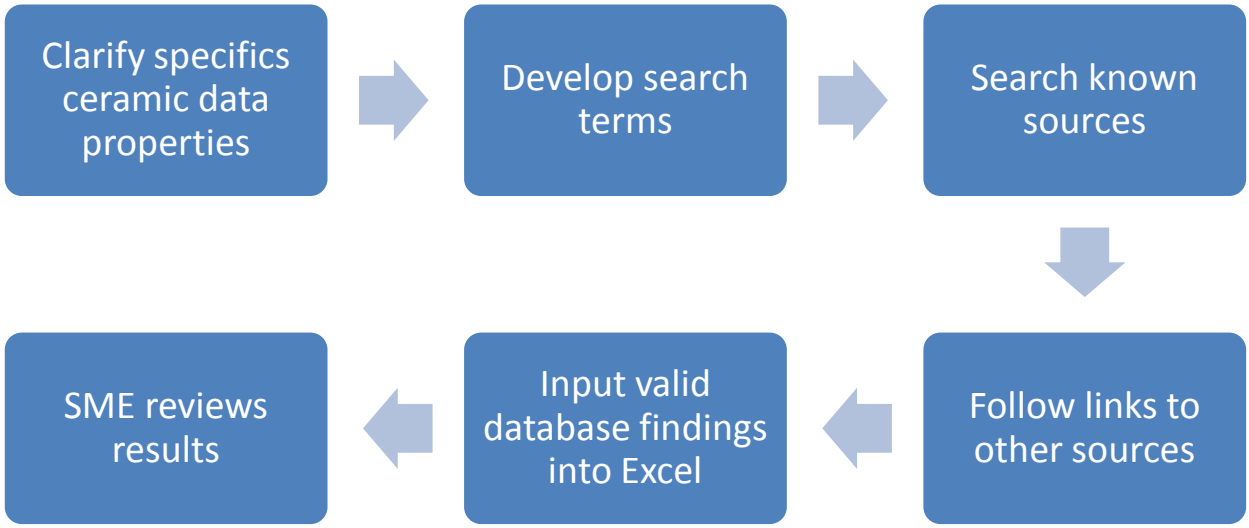

Figure 1. Schematic representation of the search strategy.

2.3 Summary of Reviewed Ceramics Data Resources

Over 100 possible ceramic property data resources were identified. Many of these contained no property data and are not included in this summary. Table 2-1 lists the ceramics data resources that do contain ceramic property data. A few of these are printed data resources or organizations with a broad mission to provide ceramic data and information. The reviewed data resources have been divided into the following categories:

- Comprehensive and General Ceramics Databases – Government and University
- Ceramic Phase Equilibria and Crystallographic Structure Databases
- Ceramic Materials Producers Databases
- Glass Databases
- Comprehensive and General Ceramics Databases - Commercial Database Providers
- Other Ceramics-related Databases
- Ceramics-related Data Publications

A brief description of each of these ceramics data resources is given in Appendix B. Where possible, we describe the extent of the data available, but for cases in which they charged a fee, we did not determine the details of the database. This list of ceramics data resources will be made available electronically to the public, as publicized in the article in the ceramics press that will be prepared.

Our general conclusions about the availability of ceramics property data are as follows.

- While considerable amounts of ceramics property data are available, no single resource is very comprehensive.
- Many of the data resources are out of date and are no longer being updated.
- Data quality indicators are lacking for most data resources.
- It is doubtful, given the effort required to locate all these data resources, that any individual ceramic scientist or engineer is aware of all or even most of these resources; this was confirmed at the E-Ceramics 2012 workshop described in Section 3.
- In aggregate, many types of properties are not adequately covered, including some fundamental types of fundamental ceramic properties.
- Performance data are incomplete, and historical coverage of these properties is lacking.
- No single point of access exists. the National Institute of Standards and Technology (U.S.) and two institutes in Japan do provide access to multiple data resources.
- Each for-fee data resource has a different fee structure: some are inexpensive and easy to subscribe to, while others are more expensive and require greater effort to subscribe.

Table 2-1. Databases and Other Data Resources Reviewed in this Report.

Name	***Builder or Maintainer***
Comprehensive and General Ceramics Databases – Government and Universities	
Ceramic WebBook	National Institute of Standards and Technology
Network Database System for Thermophysical Property Data	National Institute of Advanced Industrial Science and Technology (AIST), Japan
Materials Project	Massachusetts Institute of Technology (MIT)
Thermal Protection Systems Expert and Material Properties Database (TPSX)	National Aeronautics and Space Administration (NASA) Ames Research Center
MATBASE	Matbase Group, Netherlands
Ceramics Summary and Design Data Files (Compendium)	University of Dayton Research Institute (UDRI)
Optical Properties of Ceramics and Ceramics Thin Films	National Institute of Advanced Industrial Science and Technology (AIST), Japan
Network Database system for Thermophysical Property Data	National Institute of Advanced Industrial Science and Technology (AIST), Japan
CCDB Glaze Database	National Institute of Advanced Industrial Science and Technology (AIST), Japan
RASMIM (Raman Spectra Database of Minerals and Inorganic Materials)	National Institute of Advanced Industrial Science and Technology (AIST), Japan
Materials Database	Japan Aerospace Exploration Agency (JAXA), Japan
Mat Navi, NIMS Materials Database	National Institute of Materials Science(NIMS), Japan

Table 2-1. Databases and Other Data Resources Reviewed in this Report.	
Name	***Builder or Maintainer***
Kaye & Laby Tables of Physical and Chemical Constants	National Physical Laboratory, U.K.
Materials Properties Open Database	University of Caen Basse-Normandie, France
Mat Bank	Korea
Tribocollect	Bundesanstalt für Materialforschung und –prüfung, Berlin
Ceramic Phase Equilibria and Crystal Structure Databases	
Phase Equilibria Diagrams	National Institute of Standards and Technology and the American Ceramic Society, USA
Inorganic Crystal Structural Database (ICSD)	FIZ Karlsruhe, Germany and National Institute of Standards and Technology
Bilbao Incommensurate Structures Database	Basque University, Spain
The American Mineralogist Crystal Structure Database	Mineralogical Society of America and Mineralogical Society of Canada
WWW-MINCRYST	Institute of Experimental Mineralogy, Russian Academy of Sciences
Database of Zeolite Structures	Structure Commission, International Zeolite Association
Ceramic Materials Producers Databases (selected examples)	
Dynallox Alumina Ceramics	
Morgan Technical Ceramics	
Boston Piezo-Optics Inc.	
COORSTEK	
Du-Co Ceramics	
Accuratus	
Ceradyne	
Materials Science and Engineering, State University of New York at Stony Brook	
Properties of Piezoelectricity Ceramics	Morgan Technical Ceramics
Glass Databases	
SciGlass Property Information System	Scimatics, Newton, MA
INTERGLAD	New Glass Forum, Japan
Comprehensive and General Ceramics Databases – Commercial Database Providers	
MatWeb	MatWeb, LLC, Blacksburg VA
Thermophysical Properties of Materials Database (TMPD)	CINDAS LLC, West Lafayette IN
Microelectronic Packing Materials Database (MPMD)	CINDAS LLC, West Lafayette IN
Granta Data Series	Granta Material Intelligence, U.K.
Matereality Global Data Center	Matereality LLC, New York

Table 2-1. Databases and Other Data Resources Reviewed in this Report.	
Name	***Builder or Maintainer***
JAHM Software	JAHM Software, Inc., Reading MA
Material ConneXion Online Materials Database	Material ConneXion, New York, NY
ProQquest Deep Indexing: Materials Science	ProQuest, Cambridge Information Services, Ann Arbor MI
Materials Properties Database	Makeitfrom
efunda	eFunda, Inc., Sunnyvale CA
Other Ceramics-related Data Resources	
American Ceramic Society	
ASM International	
Mindat.org	Mindat, Coulsdon, Surrey, England
Materials Digital Library Pathway (MatDL)	Kent State University, OH
Advanced Materials, Manufacturing, and Testing Information Analysis Center (AMMTIAC)	Alion Science, Rome NY
Ceramics-related Hard Copy Data Sources	
CRC Materials Science and Engineering Handbook	Ed. By J.F. Shackelford, W. Alexander, and J. S. Park
Thermal and Other Properties of Refractories	Technical Report Program No. R056
Single Crystal Elastic Constants and Calculated Aggregate Properties: A Handbook, 2nd Edition	Ed. by G. Simmons and H. Wang
Elastic Moduli Data for Polycrystalline Oxide Ceramics	Ed. by R. G. Munro
Handbook of Optical Constants of Solids II	Ed. by E. D. Palik
Data Evaluation Theory and Practice for Materials Properties: NIST Recommended Practice Guide 960-11	Ed. by R. G. Munro

Section 3. Task 2 Results of a Ceramics Informatics Workshop

3.1 Workshop Logistics

As part of this study, 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, Virginia, on June 4th and 5th, 2012. The workshop focused on the prospects and challenges for improved access to, and quality of, ceramic property data. The goal of the workshop was to determine 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 was held free of charge, by invitation. Some of the topics discussed are as follows:

- Materials as a Key Defense Strategy
- Ceramics Databases: A Review
- Ceramics Data in Asia: A Review of Approaches
- New Approaches to Data: The Materials Genome Initiative
- Scientific Data and Social Media: Thoughts for the Future
- What are current requirements for improved access to ceramic property data?
- Which needs are unmet and which needs are most critical?
- Are people willing to pay for improved access?
- What actions are required? Who should take action? How should they be supported?

3.2 Workshop Attendees

The workshop was designed to obtain information from the user community, especially from those who have a real need for access to the latest and best data. As a result, of the thirty attendees, 14 were from industry, 14 from government laboratories and materials organizations, and 2 from academia. Attendees' names and institutions are listed below in Table 3-1.

Table 3-1, Attendees at E-Ceramics 2012.

Name	***Organization***
Industry	
Todd Steyer	Boeing Aircraft
Gary Fishman	Industrial Consultant
Alex Coletti	SM Resources Corporation
Eileen DeGuire	American Ceramic Society
Steve Freiman	Freiman Consulting
Sharon George	Springer
John Holowczak	United Technologies Research Center
Arne Knudsen	Kyocera America
Toni Marechaux	Strategic Analysis
Charles Spahr	American Ceramic Society
Karen Cavallo Miller	Information International Associates
Lora Cooper Rothen	DUCO Services
John Rumble	R & R Data Services
Alan Raynes	Konrad, Raynes, & Victor
Government Laboratories and Agencies	
Matthew Bratcher	US Army Research Laboratory
Kevin Ewsuk	Sandia National Laboratory
Jeffrey Fong	NIST
Terrell Vanderah	NIST
James Warren	NIST
Eric Wuchina	NSWC

Table 3-1, Attendees at E-Ceramics 2012.	
Name	***Organization***
Randy Hay	Air Force Research Laboratory
Ken Lipkowitz	Office of Naval Research
Lynette Madsen	National Science Foundation
Suveen Mathaudhu	US Army Research Office
James McCauley	US Army Research Laboratory
J. P. Singh	US Army Research Laboratory
Lew Sloter	DoD OASD (R&E)
David Stepp	US Army Research Office
Universities	
Laura Bartolo	Kent State University
Jim Shackelford	UC Davis

In addition to the invited talks, considerable time was allotted for group discussion, which has been summarized below.

3.3 Workshop Discussion and Conclusions

Following the daily presentations each day, roundtable discussions were held with all attendees to give all participants a chance to express their thoughts and to identify important issues that should be addressed by the ceramics data community. Major points identified included the following:

- The database of ceramics databases that has been compiled under this study and described at the workshop should be made available to organizations such as the American Ceramic Society, ASM International, and any other group that desires it to be freely available to the general public.
- A concerted effort is needed to build a high quality database of fundamental properties of single crystals to support atomistic scale modeling. Needed data include elastic constants, electrical constants, and other data regarding similar properties. The database should be freely available and 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.
- Organizations such as NIST and the American Ceramic Society should solicit ideas from the ceramics community as to the need for new data evaluation projects for ceramic property data, including performance data. This includes the possible update of the NIST Ceramics WebBook, as well as update and production of electronic classical print data compilations.
- Given the number and diversity of existing ceramic databases, organizations such as the American Ceramic Society should explore establishing a ceramics data portal that provides a single point of access to as many ceramics data resources as possible. The data portal should include visualization and other tools, as well as a comprehensive directory of content.

- Access to publicly available data is important for ceramics users and producers, as those data allow optimization to local needs.
- International Traffic in Arms Regulations (ITAR) restrictions in some cases limit sharing of data on advanced materials, especially ceramic matrix composites.
- 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.
- There should be a continuing series of materials data workshops and conferences to provide for the exchange of knowledge and fostering of progress in this area.

Section 4. Task 1a.2 - Ceramics and Materials Databases in Asia

4.1 Introduction

A major component of this project was to understand and assess activity in Asia on building and disseminating ceramics and other materials databases. To accomplish this, two subcontractors, Dr. John Rumble of R&R Data Services, and Dr. Steve Freiman of Freiman Consulting, attended the Third Asian Materials Data Symposium, held in Okinawa, Japan, and then they paid visits to numerous institutes in Shanghai and Beijing, China. The visits in Beijing were arranged by another subcontractor, the Asian Technology Information Program (ATIP).

There are many reasons why it is important to look to Asia for activity in this area. First, Japan and Korea have strong traditions in industrial advanced ceramics and have long been research leaders in this field. The newly emerging industrial economies of China and India are creating important new manufacturing capabilities, some of which are based on advanced ceramics and other materials. The entire East Asia region is making large investments in science and using R&D as a foundation to move from commodity manufacturing to higher value, specialized products. At the same time, information technology, including information science and data infrastructures, are being developed in support of the next generation industry.

These investments include significant efforts in the development of a broad range of materials databases, as reflected in the emergence of the Asian Materials Database Symposium series as the primary international conferences in this subject area over the last six years. Both China and Korea have made national commitments to building a wide variety of materials databases, and Japan continues its support, albeit less aggressively than previously.

4.2 Conclusions

Japan, China, and Korea are in different stages of maturity regarding materials databases in general and ceramics databases specifically, in terms of coverage, priorities, and available resources. Japan has sophisticated knowledge of materials databases and has been a leader in

their development and dissemination for many years. Today, however, budget constraints mean that limited resources are available, and next generation activity has been severely limited.

China, on the other hand, has money and energy and is developing an internal knowledge base of materials databases. If China links its activities more closely to industrial needs, its efforts will not only grow in size, but will also increase in impact.

Korea, in contrast, has strongly combined its materials, chemical, and ceramics database activity with industrial needs. However, Korea faces a resource problem, especially as it completes the first five-year effort with more limited progress than had been anticipated.

U.S. leadership in materials research is critical for reaching our national defense, economic, and quality-of-life goals. Further, innovation and advances in materials today require access to materials data, regardless of where those data are generated or made available. For several decades, the United States was the world's leader in materials data activities through aggressive programs implemented by government agencies, professional societies, private data companies, industrial materials producers, and standards development organizations. Our review of activities in Asia, especially those in China, Korea, and Japan, reveals that our materials data leadership is in danger of being lost if proactive steps are not taken by all interested U.S. parties.

It is clear from our review of Asian materials data activities that our leadership in materials data is within five years of being relinquished, likely by China; once lost, it will be very difficult to reclaim. For the discussion of the Asian visits detailed below. As we do so, we urge the reader to keep three aspects in mind:

- Achievements – what is actually being done, and what has been accomplished?
- Challenges – what problems are the Asian data activities facing?
- Resources – what financial support has been provided, and what are the prospects for continued or new support?

4.3 Third Asian Materials Database Symposium (AMDS)

AMDS was held in April 2012 in Naha, Okinawa, Japan, and was primarily organized by the National Institute for Materials Science (Japan). Co-organizers included the Korea Institute of Ceramic Engineering and Technology, the Korea Institute of Materials Science, the Korea Research Institute of Chemical Technology, and the University of Science and Technology Beijing. Over 100 people attended, with 69 papers presented, as summarized in Table 4-1.

Table 4-1. 3rd Asian Materials Database Symposium Country of Origin of Presentations

	Japan	China	Korea	USA	Europe	Russia	Taiwan	India	Thailand	Algeria	Vietnam	Iran
Oral	13	10	4	3	3	2	1	2	2	0	1	0
Poster	17	5	2	0	0	0	2	0	0	1	0	1

The topics covered a broad range of subjects related to materials databases and included the following:

- Impact of materials databases
- Nanoinformatics
- Major materials data systems
- Mechanical property databases
- Corrosion databases
- Computation and simulation databases
- Database development
- Interoperability

Two oral and five poster presentations on ceramics data generation and databases were made, as shown in Table 4-2.

Table 4-2 Presentations on Ceramics Databases and Data Generation at the 3rd AMDS

	Item #	*Title*	*First Author*	*Organization*	*Country*
Oral	1	Current status of ceramics bank – a ceramics materials database	Seong-Min Jeong	Korea Institute of Ceramic Engineering & Technology	Korea
	2	A perspective on materials databases	Steve Freiman	Freiman Consulting	USA
Poster	3	Inorganic nonmetallic materials database	FU Jian	Shanghai Institute of Ceramics	China
	4	NIMS Inorganic Materials Database AtomWork	XU Yibin	National Institute of Materials Science	Japan
	5	Semiconductor materials database	SHIMIZU Junya	National Institute of Materials Science	Japan
	6	Prediction of Si/GE thermal boundary resistance by non-equilibrium molecular dynamics	MINAMOTO Satoshi	Techno-Solutions Corporation	Japan
	7	Effect of micro-detonation of striking arc machining on	TIAN Xinli	Academy of the Armored Forces	China

Table 4-2 Presentations on Ceramics Databases and Data Generation at the 3rd AMDS					
	Item #	***Title***	***First Author***	***Organization***	***Country***
		microstructure for silicon nitride ceramics		Engineering	

The first five papers in Table 3-2 provided overviews of the major ceramics database activities in Asia and the United States, which are described in more detail in Section 2 of this report. Some general conclusions, however, should be pointed out in this discussion about Asian activities. First, the mere existence of AMDS demonstrates a shift of interest in materials data from the United States and Europe to Asia. Many attendees were younger and saw data work as an integral part of becoming a materials researcher.

With the exception of Korea, as discussed below, most of the database reports concerned individual efforts, which might be part of a larger program (e.g., the China Materials Data Sharing Network). These efforts were generally uncoordinated, especially with respect to scope, metadata standards, historical coverage, and properties included. There was virtually no mention of standard formats and the mechanics of data sharing.

4.4 Japan

The focus of materials data activity in Japan has consolidated at the National Institute of Materials Science (NIMS), which has made an institutional commitment to leadership in Japan. As described in Section 2, NIMS has developed a portal to many Japanese-based materials databases, many of which have been developed over the last several decades without being part of a central plan. The coverage is disparate, and there appear to be no broad coverage goals. Many of the databases, however, do have English language interfaces. Japan does not maintain ongoing government-funded materials data centers, and as the initial leaders of the Japanese materials data community approach retirement, university and federal data activities are being curtailed.

One exception was described by Kohmei Halada in a talk about GENSO-SENRYAKU (strategic elements' design) that focused on reduced consumption of critical materials through improvements in materials efficiency, substitution, and recycling. Much of the emphasis of this project is on new materials design from "electronic structure control" (their term), which is basically computational materials design starting at the atomic level. The NIMS AtomWork database supports this first-principles data modeling effort. An additional focus is on nanomaterials, but few details were given.

Japanese researchers have long sought to push first-principles materials design and AtomWork as the successor to the Pauling File, which combined crystallographic, thermodynamics, and atomic property data into one resource linked to a variety of software models. It is not clear whether any new materials have been successfully designed and developed using this approach.

In spite of their long history with advanced ceramics, the Japanese have not put special emphasis on ceramics databases, but rather on materials databases in general.

4.5 Korea

Because of the presence of many Korean materials data experts at the Third Asian Materials Data Symposium, as well as significant government investment in large scale materials data programs, an analysis of the situation in Korea was added to provide additional perspective on Asian activities.

In 2007, Korea began its Standard Reference Data Program and launched three major efforts to support Korean industry with large-scale, comprehensive databases: one each on chemicals (especially polymers and specialty chemicals), metals, and ceramics. Each of these systems was described in detail at the 3rd AMDS. In spite of what seem to be significant investments, none of the systems has reached maturity, and the coverage (in terms of number of materials, historical content, and amount of data) is still rather limited. At present, interfaces are primarily in Korean-language only. While support has been substantial, the typical problems of making data uniform and harmonized have been more costly than anticipated. In a meeting of several project leaders with Rumble and Freiman, the Korean managers described the great uncertainty of future funding when the initial five-year program ends later this year. (Note: It was just learned [late October 2012] that the three Korean database projects on ceramics, metals, and chemicals have been extended until 2016.)

4.6 China

Visits were made to institutes in Beijing and Shanghai that are actively involved in materials data activities in general and ceramics research specifically. The major ceramics research organization in China is the Shanghai Institute for Ceramics, part of the Chinese Academy of Sciences (SICCAS). SICCAS has over 600+ researchers engaged in virtually every area of ceramics research, including the following:

- High Performance Ceramics and Superfine Microstructure
- Structural Ceramics Engineering
- Inorganic Coating Materials
- Information Materials and Devices
- Biomaterials and Tissue Engineering
- Energy Materials
- Artificial Crystals
- Ancient Ceramics

During an afternoon-long meeting with senior leaders of SICCAS, we reviewed their database activities in detail. Presently SICCAS has a small database effort focused almost exclusively on saving their internal research results. SICCAS is part of the China National Materials Data Sharing System, but based on our meeting with them, they have not made much progress in putting any databases on this network.

SICCAS is very concerned with data quality and uses high quality databases such as the Inorganic Crystal Structure Database (USA-Germany) and the databases of the International Centre for Diffraction Data (USA). They do not, however, have any specific data evaluation

efforts except in the context of specific research results. Most importantly, at the present time, SICCAS does not have plans to capture existing ceramic property data in any systematic way.

Because of our proximity to Beijing, one of us (Rumble) worked with the Asian Technology Information Program (ATIP) to visit organizations in Beijing working on materials data, as listed in Table 4-3. The visits were arranged by local representatives of ATIP, a subcontractor on this project. ATIP's extensive knowledge of local research groups and university infrastructure contributed to the success of these visits.

Table 4-3. Beijing Organizations Working on Materials Data Visited During This Trip.

Organization	***Department***	***Data Type***
University of Science and Technology Beijing	Computer Science and Communication Engineering School; Materials Safety Center, Department of Materials Science	Materials safety and reliability, corrosion data, and general materials property data
Chinese Materials Research Society		Organizer of meetings on materials data
Chinese Computer Network of Information Center	Chinese Academy of Sciences	China National Materials Data Sharing System
Chinese Nanotechnology Center		Small effort on nanomaterials data
Beijing University of Technology	Department of Materials Science	Rare earth property data
Tsinghua University	Department of Ceramics	No data activity

We start with the China National Materials Data Sharing System (CNMDSS), whose goal is to build an integrated materials data sharing network for China; many of the important materials data activities in China are part of this effort. CCNMDSS is one of 14 components of China's key infrastructure projects, which is now in year five of six years of funding. The project is led by the Chinese Computer Network of Information Center (CCNIC), which is part of the Chinese Academy of Sciences and associated with the Chinese CODATA National Committee. Among the materials areas, where databases are being funded, are ceramics (SICCAS) materials safety and reliability, corrosion data, and rare earth data, as shown in Table 3-3.

Despite announced plans, there is only limited activity on ceramics data, which is being carried out by SICCAS. It is interesting to note that Tsinghua University, one of China's leading university ceramics research groups, has virtually no data activity.

The initial activities for other projects have focused on capturing internal research results generated by individual research groups. There are no real efforts to develop standard data formats or metadata, and when asked, none of the groups had plans to capture old data or existing data sets, nor did they plan to have complete coverage in terms of either materials or properties. It should be noted that within these individual materials science research groups, the data activities have very broad participation from students, post-docs, and younger faculty

members. There clearly is an interest to nurture materials informatics, but as yet, that interest has not matured in a cohesive, planned activity.

At the University of Science and Technology Beijing, great emphasis is being placed on research into materials safety and reliability, and the three groups with whom we met all placed emphasis on using the CNMDSS as an important tool to disseminate their research results. One interesting aspect of our conversations is that virtually none of the groups was aware of previous materials database work in the United States or Europe, though there was knowledge of work going on in Japan. Consequently, the Chinese groups are facing some of the same problems U.S. and European efforts faced in the 1990s, including the following:

- Materials are constantly changing, and property data for older materials becomes less relevant as new materials are developed.
- Standard for formats or metadata are limited or nonexistent.
- Integration of disparate databases built and controlled by different parties is difficult.
- Funding is for an initial six-year period, with no guarantee that all projects will be renewed in the second six-year period.
- Virtually no foreign data are being collected or included.
- There is limited linkage to industry (though this was less of a problem in the United States).

In conclusion, China has adequate funding to complete the National Materials Data Sharing System as originally conceived, but it is unclear whether it has the dedication and resources to make it comprehensive or to maintain it over the long term. In spite of its lack of knowledge about specific Western materials databases and data systems, China is using modern networking and database technology. China appears to be successful in engaging next generation materials scientists and engineers, but it has virtually no thoughts about using social media for increasing the scope of dissemination or impact of their investments. Officials at the Chinese Computer Network of Information Center who are overseeing the National Materials Data Sharing Network said that work is spreading to groups outside Beijing and Shanghai.

It was just learned (late October 2012) that the China Materials Data Sharing Network program will be reviewed, and new and renewal projects will be chosen to start in 2014. The present program covers six branches of materials data and has a total budget for the first six-year program of 60M Renminbis, or 10M Renminbis per year. Taking into account the lower cost of research in China as compared to the United States, we believe this is equivalent to at least $6M per year.

Section 5. Task 1B Options for Developing Models for Providing Web-based Access to Ceramic Property Data

5.1 Introduction

The last twenty years has seen a rapid maturing of the World Wide Web as the primary mechanism for providing access to all types of information, including the properties of ceramics materials. While in the early years of the web, the emphasis was on free access, but the potential for commercial web uses has emerged, and today an incredibly rich diversity of commercial services complement the no-fee services. In this section, we discuss various options for developing models for web-based access to ceramic property data.

5.2 Basic Data Access Process Model

Our model for this discussion is illustrated in Figure 2. We have divided the entire data access process into three components: users, data resource builders, and the data access providers that link the two together. Feedback loops between the components are critical to ensuring that needed services and products are provided.

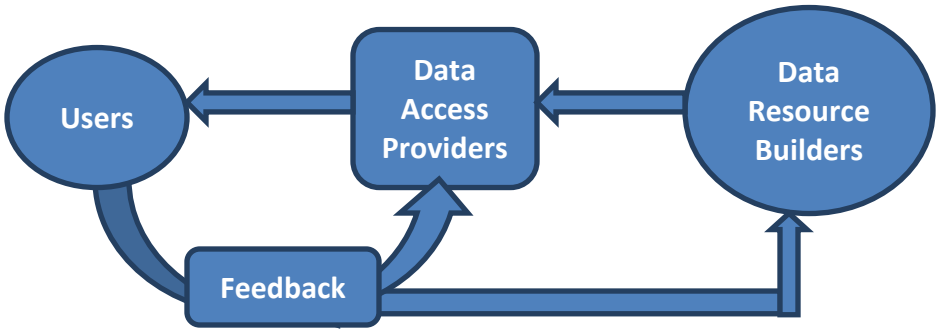

Figure 2. The basic data access process model.

It is instructive to begin from the user perspective, to ask, *what does a user of ceramic property data need, want, and expect?* The answers to these questions can be summarized as follows.

1. **What is needed?** Access to property data for newest materials, as well as fundamental properties of all materials
2. **What is wanted?** Quick and easy access, with the minimum fuss, through the smallest number of access points possible
3. **What is expected?** Lowest possible costs, systems that always provide answers as advertised, with 100% availability and highest quality or provenance indicators

From the perspective of those who build data resources, the questions as follows:

1. **How do we preserve generated data (from experiments, calculations, compilation) easily and accurately?** Through use of modern, easy-to-use database tools

2. **How can these data be made available to those who need them?** Through use of the World Wide Web
3. **How can the data collection and preservation effort be supported?** Through government or private sector subsidies or fee-based services

These two communities are linked by the data access providers. These are organizations, non-profit and commercial, that provide access to data as a free service, for profit, or both. Types of data access providers found in the world of materials data in general, and ceramics data in particular, and their characteristics, are listed in Table 5-1 below.

Table 5-1 Types of Data Access Providers

Organization Type	***Characteristics***	***Example(s)***	***Types of Charges***
Professional Societies	Organized around a discipline or special interest; membership usually limited to specialists in a field; provides data as a service to its members	America Ceramic Society, ASM International	Fee-based services
Commercial Data Services (Multi-disciplinary)	Companies that provide data in a variety of fields, sometimes not even related to science and technology; often former publishers	Springer-Verlag, CRC Press	Fee-based services
Commercial Data Services (Specialized)	Companies that provide data in a few disciplines (usually related); often provide tools to exploit the data	Granta	Fee-based services
Web Search Services	General web search engines that can find all types of information	Google, Yahoo, Bing	Free
Materials Producers	Companies that make materials and provide data about their materials products	Kyocera	Free
Government Agencies	Government agencies that maintain data programs either in many disciplines or to support specific missions	NIST (General S&T data), DoD (many types of materials data; DOE (mission specific data)	Mostly Free, but NIST has authority for fee-based services

Table 5-1 Types of Data Access Providers

Organization Type	***Characteristics***	***Example(s)***	***Types of Charges***
Universities	Academic organizations that make available data produced by their research groups either under a single grant or from a series of related projects		Free and fee-based services
Research Institutes	Non-profit research organizations that make available data produced by their research groups either under a single grant or from a series of related projects		Free and fee-based services
Non-profit Data Organizations	Organizations established to collect and provide access to special types of data, usually spun off from other organizations	International Centre for Diffraction Data	Free and fee-based services
Materials Advocacy Organizations	Groups that promote the use of specific materials	Aluminum Association; American Iron and Steel Institute	Generally free

The question now becomes, do these data providers have the motivation to provide access in a manner that meets user needs, as listed above, or in a manner that meets the needs of those building data resources? For ceramic property data, based on the analysis we have given in Section 2 describing present-day available ceramics data resources, the answer is ***no***. In fact, most data providers do not seem to want to provide access to any data resources besides their own. They do not want to make access to multiple data resources easy, quick, or through a single point of entry. The exception might be commercial data providers, but to date, none has provided access to many ceramic data resources though a single data portal. Given the numerous data resources and the difficulty a single user would have in knowing about and using multiple resources, it seems that individual providers of ceramic data resources want to keep the present system.

There are a number of reasons why these data resource builders and data access providers do not serve the ceramics data user community adequately today in terms of providing access to multiple data resources, including the following:

- Small number of potential users
- High cost of building and maintaining a comprehensive system
- Poor understanding of benefits and revenue streams
- Labor-intensive nature of building and maintaining scientific and technical data collections

- Variability of ceramics properties due to small changes of composition, processing, or manufacturing
- Expense of data evaluation and curation
- Lack of standardization of ceramic materials
- Rapid innovation leading to new materials

At E-Ceramics 2012, the ceramics informatics workshop held in June 2012 as part of this study (see Section 5), the difficulty in learning about ceramics data resources and gaining access to them was highlighted as a major concern of the user community. ***In particular, participants were generally unaware of the multitude of ceramics data resources presently available, and even if they knew about a resource, contractual and fee arrangements posed significant barriers to use***.

The preponderance of challenges to those who build and provide access to ceramics data resources combine with the challenges faced by the ceramics data user community combine to make the present-day situation unsatisfactory. The goal is to identify and understand these challenges so that access to needed ceramic property data will improve significantly over the next decade.

5.3 Options for Developing Models for Providing Web-Based Access to Ceramic Property Data

Based on the opinions expressed by attendees at the E-Ceramics workshop 2012 (Section 3), user needs for access to ceramic property data are not being met. How best can interested parties—industrial product designers, component manufacturers, and government agencies—plan to meet those needs? First we must recognize that ceramic property data are important enough to industrial and government designers and engineers so that they have historically been willing to pay for data handbooks, individual databases, and research programs to gain access to needed data. 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, non-linear process that results in commercial products or materials. Property data are often critical in the ***early*** stages of product conceptualization and design, so that the time separation between data usage and release of a product is usually several years. The conundrum is that the value of property data is recognized, but its importance in the economics of a final product is underestimated.

In addition to these considerations is the fact that properties of engineering materials, especially ceramics, are highly variable in terms of small compositional, processing, and manufacturing changes. Many ceramics are individually tailored by a single company to specific product needs. A specific ceramic is unlikely to be reproduced by other companies. As a result, ceramic property data are important for determining general materials selection, but they often involve significant fine tuning before a final selection is needed.

Consequently, responsibility for meeting the needs of a general user of ceramic property data is not clear cut. Professional societies, which collectively are a major provider of materials property data in the United States, do not feel the pressure to provide 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. While small commercial data providers claim to provide comprehensive coverage, in fact, their data products are outdated, incomplete, or both. Ceramics manufacturers are interested in advancing only their materials.

How can the ceramics data user community coalesce and provide a coherent argument for meeting their needs? Based on activities in other scientific and technical disciplines, several potential approaches have been identified that are discussed below.

- ***Informal action of the user community through workshops and articles in materials and informatics press***

  In many areas, such as astronomy, grass-roots efforts have succeeded, primarily because individual scientists recognized the value of having coordinated data activities, and they also recognized that the limited *economic* value of their data precluded fee-based services. As a result, once grass-roots efforts reached a certain level of activity, researcher funders came on board and provided the needed subsidies.

  Ceramics property data are important to ceramic producers who use data to differentiate and sell their products. They are also important to product manufacturers who use data to produce better engines, electronics, etc. This high economic value complicates and inhibits grass root efforts to provide better access. Ceramics producers want to control their proprietary data; manufacturers who use ceramics data do not want to share data in order to maintain market share.

- ***Professional societies or industrial organizations should be approached to establish new ceramics data activities.***

  For over a century in the United States, professional societies and industry associations have been primary mechanisms for industrial firms to cooperate in sharing technology, information, and data. Many of these organizations routinely provided quality data products and services in the form of publications, handbooks, and data tables, usually but not always on a fee basis. In fact, for many groups, the income from these products helps support other activities.

  Over the last three decades, professional societies in particular have had to confront moving into the information age, and with the World Wide Web and internet, they have struggled to develop data services that were revenue neutral, at a minimum. The size of the perceived initial investments, as well as the lack of a fee structure that would be accepted, is still a challenge today, resulting in far fewer online data services than might be expected. It has been easier to maintain the status quo rather than to take big risks, especially for many societies for which membership has been declining through the recent financial crisis.

One goal of this work is to alert professional societies interested in ceramic property data to see that significant opportunities exist for providing new and important services to their members and others by providing better access to those data.

- ***The Federal Government should fund an independent review of access to ceramics data to identify the problem and propose solutions.***

  Beginning in the late 1970s, a large number of studies and reviews of the opportunities associated with computerized materials data have been undertaken, some of which led to the establishment of the fairly short-lived National Materials Property Data Network. The issues faced by the data community today have been well recognized and studied. Further review is unlikely to lead to immediate action. The challenges to U.S. leadership in terms of its materials capabilities, however, are another matter. As other countries, especially China, continue to invest heavily in an informatics future, U.S. industrial, economic, and security competitiveness must be scrutinized. Advanced materials play a critical role in our competitiveness, and periodic assessments of the issues are needed to ensure that we maintain our world leadership. It must be recognized, however, that such studies and reviews are more important for government actions rather than private sector investments. As a result, improvements in access to ceramic property data by the private sector (industry, professional societies, and information industries) are less likely to result.

5.4 Potential Business Models for Web-based Access to Ceramic Property Data

To review briefly what users want:

- They want web access to as much ceramic property data as possible.
- They want access to be as easy and quick as possible.
- They want to know the quality of what they are accessing.

In terms of having a single point of access, the two business model ***extremes*** are as follows:

1. A single, monolithic ceramics data system is established with data from as many sources as possible in the system in a uniform format and a single interface. A single license is needed.
2. A federated ceramics data system is established with a single point of entry, with the user having to contract with each data resource available in the system and with multiple interfaces.

Neither approach is likely to be viable. The cost of building a monolithic data system is significant, even with all the advances made in information technology and web technology over the last twenty years. No standards exist for describing ceramic materials or ceramic property data. The effort to integrate data from the more than 50 ceramics data resources identified in this report is daunting and not economically feasible. Many of the data resources are proprietary and are designed to make money for their builders or providers. These have little economic incentive to cooperate with a monolithic system.

A federated system with a single point of entry, but with multiple user interfaces and requiring users to contract individually with each resource, is essentially the system in place today, with Google, Yahoo, or other search engines acting as the single entry point, and with linkage to each identified data resource the responsibility of each individual user. Today's system is unsatisfactory from many points of view, not the least of which is the lack of selectivity among search results. 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, the contents cannot be understood until contracts are in place.

A more workable business model lies between the two extremes defined above. A robust ceramics data system that inherently meets user needs is a hybrid federated system. In this model, there are multiple points of entry via multiple systems, depending on the market place. Each system would be similar in many respects and would likely include the following characteristics:

1. A single access point, commonly referred to as a data portal, would be available and 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 would initially 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 success of such a business model depends on the willingness of a system provider to (1) include the greatest possible number of data resources in its system and (2) to negotiate contracts that provide adequate revenue to each data resource and to the system provider. Given the existing recognition by the user community of the economic value of ceramics materials data, the willingness to pay is not lacking. Instead, the major hurdles are (1) knowing that a data resource exists, (2) knowing the actual contents of each data resource, and (3) the difficulty of negotiating contracts with multiple data access providers.

While some private sector organizations have attempted to develop a comprehensive materials data system, none have tried to do this for ceramic property data alone. From the perspective of today's users, as described throughout this report, many data resources are unknown, and access can be difficult. The need for one or more single points of entry (data portals) to multiple existing data resources is clear, and the opportunity to use current tools to create such a system is there. With more than 50 data resources available today, coverage in terms of materials and properties is ***likely*** sufficient to attract a sufficient number of users to generate the revenue

necessary for a sustaining system. Before investing in such a system, any organization seriously embarking on this path would need to conduct a detailed user survey and would also need to negotiate with data resources.

The role of the government in designing, building, operating, or even advocating such a system is limited. The government's does build individual data resources needed for its missions, but the government also can and should work with interested parties to help them overcome barriers in making government-funded data widely available on such a system.

Appendix A

Workshop Agenda

Workshop on E-Ceramics
Prospects and Challenges for Improved Access to Ceramics Property Data

Arlington VA
June 4-5, 2012

4 June 2012

8:00 am	Registration and Coffee
	Opening Session
8:45 am	Participant introductions
9:00 am	Background and Workshop Goals – Steve Freiman
	Keynote I
9:30 am	Materials as a Key Defense Strategy – Lew Sloter – DDR&E
	Session 1
9:50 am	Matthew Bratcher - Army Research Laboratory
10:15 am	Coffee
10:35 am	Randy Hay – Air Force Research Laboratory
11:00 am	Ali Sayir – Air Force Office of Scientific Research
11:25 am	Kenneth Lipkowitz- Office of Naval Research
11:50 am	Box Lunch (provided)
1:00 pm	Lynnette Madsen – National Science Foundation
1:25 pm	Kevin Ewsuk - Sandia National Laboratory
1:50 pm	Todd Steyer – Boeing Aircraft Company
2:15 pm	John Holowczak -United Technologies Research Center
2:40 pm	Jim Shackelford - University of California at Davis
3:05 pm	Coffee
	Session 2
3:25 pm	Ceramics Data in Asia: A Review of Approaches - John Rumble – R&R Data Services

Session 3 - Short (10 min.) Presentations

4:00 pm	Various
5:30 pm	End of Day

5 June 2012

8:00 am	Coffee
	Keynote Talks II
8:30 am	New Approaches to Data: The Materials Genome Initiative – James Warren – NIST
9:00 am	Scientific Data and Social Media: Thoughts for the future – Alex Coletti - SMRC
	Session 4
9:30 am	Arne Knudsen – Kyocera Corporation
9:55 am	Lora Cooper Rothen – DUCO Ceramics
10:20 am	Coffee
	Plenary Discussion
10:40 am	What are today's requirements for improved access to ceramics property data? Which needs are unmet, and which needs are most critical? Are people willing to pay for improved access? What actions are required? Who should take action? How should they be supported?
12:00 noon	Working Lunch (Box Lunch provided)
1:00 pm	***Summary and Next Steps***
2:00 pm	Adjourn

Appendix B

Review of Selected Data Resources

B.1 Introduction

Each of the data resources included in Table 2-1 was carefully reviewed with respect to its content, currency, accessibility, and other parameters. The results of the reviews are given below. The data resources have been categorized as follow.

- Comprehensive and General Ceramics Databases – Government and University
- Ceramic Phase Equilibria and Crystallographic Structure Databases
- Ceramic Materials Producers Databases
- Glass Databases
- Comprehensive and General Ceramics Databases - Commercial Database Providers
- Other Ceramics-related Databases
- Ceramics-related Data Publications
-

B.2 Comprehensive and General Ceramics Databases – Government and University

Ceramic WebBook
National Institute of Standards and Technology
http://www.ceramics.nist.gov/webbook/evaluate.htm

This site provides links to three NIST ceramics databases (High-Temperature Superconducting Materials Database, Structural Ceramics Database, and Property Data Summaries that includes oxide glasses), as well as links to other ceramic information resources. The databases are searchable by author, chemical family, structure type, properties, and publication information. Search results include bibliographic citation(s) and specific property data mentioned in the original publication(s). While most of the data were not evaluated in terms of providing uncertainty bands on the property values, the databases were examined by experts to ascertain whether the experimental methods used to acquire the data were acceptable. Unfortunately, no new data have been added to this site for many years. Access is free.

Network Database System for Thermophysical Property Data
National Institute of Advanced Industrial Science and Technology (AIST), Japan
http://riodb.ibase.go.jp/

This database is maintained by AIST in Japan and contains over 9,000 sets of thermophysical property data on a variety of materials including ceramics, of which over 3,000 are available free of charge. Property data include thermal conductivity and diffusivity, heat capacity, density, vapor pressure, and others for liquids and solids. Measurement techniques are described.

Materials Project
Massachusetts Institute of Technology (MIT)
http://materialsproject.org/

This database was created by Professor Gerbrand Ceder at MIT and Professor Kristin Persson at Lawrence Berkeley National Lab. It is a database of computed properties of materials. One is able to calculate phase diagrams, crystal structures, as well as other properties. Access is free.

Thermal Materials Properties Databases
NASA Ames Research Center
http://tpsx.arc.nasa.gov/

The database was designed for analysts and engineers in the aerospace field. It is free but requires registration. It is supported by the Thermal Protection Materials & Systems Branch of the NASA Ames Research Center. It contains thermal and physical property data on a wide variety of thermal protection materials, including ceramics, ceramic coatings, and ceramic composites. Access to some of the data is restricted.

MATBASE
Matbase Group, Netherlands
http://matbase.com

Matbase claims to have the largest collection of material properties on the web. It includes physical, mechanical, and environmental properties of a large collection of materials including ceramics. The database is based on the Idemat Database at the Delft University of Technology in the Netherlands. Data can be contributed, and there is forum where questions can be posted. Sources of the data are unclear. Access is free.

Ceramics Summary and Design Data Files (Compendium)
University of Dayton Research Institute (UDRI)
http://www.udri.udayton.edu/EnergyTechnologiesAndMaterials/AdvancedHighTemperatureMaterials/Pages/CeramicsSummaryandDesignDataFiles.aspx

These data were collected through funding provided by the Department of Energy through the Oak Ridge National Laboratory. There are mechanical property data on a number of silicon carbide and silicon nitride formulations available as spreadsheet files. The data date from 1998 and do not appear to have been updated. Access is free.

Optical Properties of Ceramics and Ceramics Thin Films

National Institute of Advanced Industrial Science and Technology (AIST), Japan
http://riodb.ibase.aist.go.jp/opcc

This database contains optical properties data, e.g., reflectance, transmission for a variety of ceramic materials. Access is free.

Network Database System for Thermophysical Property Data
National Institute of Advanced Industrial Science and Technology (AIST), Japan
http://riodb.ibase.aist.go.jp/TPDB

This database is run by AIST and contains data on thermal conductivity, thermal diffusivity, heat capacity, density, surface tension, and vapor pressure for liquids, solids, and melts. Access is free.

CCDB Glaze Database
National Institute of Advanced Industrial Science and Technology (AIST), Japan
http://riodb.ibase.aist.go.jp/ccdb

This database contains data on ceramic glazes such as visual appearance, composition, and firing conditions. They eventually expect to have data on 50 thousand pieces. Access is free.

RASMIM (Raman Spectra Database of Minerals and Inorganic Materials)
National Institute of Advanced Industrial Science and Technology (AIST), Japan
http://riodb.ibase.aist.go.jp/rasmin

This is a database of Raman spectra for a wide variety of materials. Access is free.

Materials Database
Japan Aerospace Exploration Agency (JAXA), Japan
http://matdb1n.tksc.jaxa.jp/MaterialEvaluation/

This database is maintained by the Japanese Space Agency. It summarizes evaluation data of materials used for space applications such as thermal control coatings, adhesives, thin films, etc. Effects of irradiation by UV, atomic oxygen, and other beams are included. Access is free.

Mat Navi; NIMS Materials Database
National Institute of Materials Science(NIMS), Japan
http://mits.nims.go.jp

This site leads to a number of separate databases on inorganic materials (AtomWork), diffusion (Kakusan), and superconducting Materials (SuperCon) as well as considerable data on metals. Access to all of their databases is free, but registration is required.

Kaye & Laby Tables of Physical and Chemical Constants
National Physical Laboratory, U.K.
http://kayelaby.npl.co.uk/

The Kaye and Laby Table of Physical and Chemical Constants is over 100 years old and has recently been made available in a web edition. It is managed by the National Physical Laboratory in the U.K. It contains a myriad of data, formulae, graphs and charts, ranging from fundamental

constants to data on fiber optics, superconductivity, etc. A number of material properties for glasses and ceramics are included. Access is free.

Materials Properties Open Database
University of Caen Basse-Normandie, France
http://www.materialproperties.org/data/

The database is searchable by properties and contains optical, piezoelectric, magnetic, and elastic data for a significant number of ceramic materials. The data were extracted from publications and are unevaluated. Access is free.

MatBank
Korea
http://matbank.org/

The Ceramics Materials component of MatBank has data on 1,016 ceramic materials with over 400 different types of properties. The user interface is in both Korean and English. The database is free to use after registration. It also has links to the MatNavi data system operated by the National Institute of Materials Science in Japan. From 2012 to 2017, MatBank is planning to include more data from international sources.

Tribocollect
Bundesanstalt für Materialforschung und -prüfung, Berlin
http://www.bam.de/php/tricot/tricot_voll.php

This database contains over 15,000 records of tribological data for materials. It was developed by the Federal Institute for Materials Research and Testing (BAM) in Germany. There is a fee to access.

B.3 Ceramic Phase Equilibria and Crystal Structure Databases

Phase Equilibria Diagrams
National Institute of Standards and Technology and the American Ceramic Society, USA
http://ceramics.org/publications-and-resources/phase-equilibria-diagrams

This is an extensive collection of phase diagrams for two, three, and multicomponent ceramic systems. It also contains salts, chalcogenides, and semiconducting compounds. The original data taken from published sources were reviewed for correctness, and suggested changes in the published diagrams were made. A senior editor subsequently reviewed all contributions. Books or CDs can be purchased through the American Ceramic Society or through NIST. NIST also has a significant number of unreviewed diagrams on file.

Inorganic Crystal Structural Database (ICSD)
FIZ Karlsruhe, Germany and National Institute of Standards and Technology
http://fiz-karlsruhe.de/icsd/html

This database contains over 150,000 crystal structures for inorganic materials. It is maintained in cooperation with NIST, who performs much of the evaluation on the entries. It is searchable by

structure type. There is a demonstration version, but full access requires a fee dependent on the type of customer and the type of access.

Bilbao Incommensurate Structures Database
Basque University, Spain
http://158.227.21.14/instrdb/

This database of incommensurate structures currently contains 89 entries. The data were taken from publications in Acta Crystollagraphica. The stored data were checked for inconsistencies. It is free but requires log in.

The American Mineralogist Crystal Structure Database
Mineralogical Society of America and Mineralogical Society of Canada
http://www.minsocam.org/msa/crystal_database.html

This database comprises every crystal structure published in the *American Mineralogist*, *The Canadian Mineralogist*, *European Journal of Mineralogy and Physics*, and *Chemistry of Minerals*, as well as selected data from other journals. The database is maintained by the Mineralogical Society of America and the Mineralogical Association of Canada and is financed by the National Science Foundation. Access is free.

WWW-MINCRYST
Institute of Experimental Mineralogy, Russian Academy of Sciences
http://database.iem.ac.ru/mincryst/index.php

This is crystallographic and crystallo-chemical database for minerals and their structural analogues. The data on minerals have links to crystallography, crystal structures, x-ray powder diffraction, chemical composition, and physical and optical properties. There are a number of other links on the site. Access is free.

Database of Zeolite Structures
Structure Commission, International Zeolite Association
http://www.iza-structure.org/databases/

This database provides structural information on all of the zeolite framework types that have been approved by the Structure Commission of the International Zeolite Association. It includes descriptions and drawings of each framework type, animated displays, crystallographic data, and simulated powder diffraction patterns. Access is free.

B.4 Ceramic Materials Producers Databases (selected examples)

Dynallox Alumina Ceramics
http://dynacer.com/PDF/dynalloxproperties.pdf

Dynallox is a commercial producer of alumina ceramics. Mechanical and thermal property data of its product are provided.

Morgan Technical Ceramics
http://www.mtcmaterialscomparator.com/

This database provides information on materials produced by Morgan Technical Ceramics. No test procedures are provided. Data are available on a number of ceramics, including aluminas, magnesia, silica silicon carbide, silicon nitride, and zirconia.

Boston Piezo-Optics Inc.
http://bostonpiezooptics.com

This database provides relevant data on their piezoelectric and optical materials such as PZT, lithium niobate, and quartz.

COORSTEK
http://www.coorstek.com/resource-library/library/8510-1042_ceramic_material_properties.pdf

COORSTEK provides a list of the properties of the materials that it produces, including alumina, silicon carbide, mullite, porcelain, silicon nitride, and zirconia.

Du-Co Ceramics
http://du-co.com/properties

Du-Co is a ceramic producer manufacturing steatite, forsterite, alumina, etc. It provides a data sheet of their products' properties.

Accuratus
http://accuratus.com/

Accuratus is a commercial entity supplying a variety of ceramic materials, e.g., silicon nitride, silicon carbide, zirconia, boron nitride. Mechanical property data are provided, along with some thermal and electrical properties.

Ceradyne
http://www.ceradyne.com/

Ceradyne manufactures a wide variety of ceramic materials, including silicon nitride, silicon carbide, boron carbide, etc. Mechanical property data on their materials are provided.

Materials Science and Engineering, State University of New York at Stony Brook
http://www.matscieng.sunysb.edu/other4.html#manufact

This site provides a list of companies specializing in materials and has a significant list of such companies who deal with ceramics. Each of these likely has material property data sheets.

Properties of Piezoelectricity Ceramics
Morgan Electronic Ceramics
http://traktoria.org/files/sonar/piezoceramics/morgan/properties_of_piezoelectric_ceramics_(pzt-4_pzt-5a_pzt-5h_pzt-8).pdf

Even though these are commercial materials, this database is included here because it is a comprehensive compilation of the properties of PZT materials. It was originally compiled by researchers at Vernitron, one of the major producers of these materials.

B.5 Glass Databases

SciGlass Property Information System
Scimatics, Newton, MA
http://www.sciglass.info/

This site contains an extensive collection of glass forming data and glass property information. SciGlass 7.1 contains data for more than 360,000 glass compositions, including more than 16,000 halide and about 35,000 chalcogenide glasses. It also provides property predictions and calculations. There is a 30-day free trial period, after which the cost can be as much as $4500/year, depending on the kind of business and license.

INTERGLAD
New Glass Forum, Japan
http://www.newglass.jp/interglad_n/gaiyo/info_e.html

This is a non-profit organization of the private sector under the jurisdiction of the Ministry of Economy, Trade, and Industry in Japan. There are about 300,000 data sets on glass structure and a wide variety of properties. The data were taken from literature sources, and no further evaluation was provided. The database is searchable. The site also contains expressions for prediction of properties. The INTERGLAD web site contains two extensive reviews of the product by respected glass scientists. There is a trial edition available. The cost of full access depends on the type and extent of the edition desired. The site was last updated in 2010.

B.6 Comprehensive and General Ceramics Databases - Commercial Database Providers

MatWeb
MatWeb, LLC, Blacksburg VA
http://www.matweb.com

MatWeb is a commercial database provider. The database contains over 8000 entries for ceramics including various forms of carbon. Access is free of charge. There is a premium search feature available for $99/year. The database contains property data on a wide variety of oxides, carbides, and nitrides, as well as data on glasses and several different naturally occurring minerals. A number of properties, such as elastic modulus, strengths, hardness, fracture toughness, etc., are presented, as well as some thermal properties, such as the coefficient of thermal expansion. The data are taken from the literature and from manufacturer sources. Test procedures are not given, so it is not possible to determine the accuracy of the data. In some cases, the table lists vendors of given materials.

Thermophysical Properties of Materials Database (TMPD) *Microelectronic Packing Materials Database (MPMD*)
CINDAS LLC, West Lafayette IN
http://cindasdata.com/

CINDAS LLC provides what it terms as critically evaluated materials property for thermal, mechanical, electrical, physical, and other properties of materials, with data on 5,000 materials. The MPMD databases focus on electronic packaging materials. The TPMD materials database contains thermophysical properties of a number of ceramic materials. There is a cost to subscribe, which depends on the number of locations and number of potential users at each location.

Granta Data Series
Granta Material Intelligence, U.K.
http://grantadesign.com/products/data

Granta is a commercial data provider with numerous data collections obtained from other sources, as well as software tools to estimate other properties. Its collection of ceramic data is relatively extensive but does not appear to be evaluated. In order to access the data, one must have a license, which can be $3000 or more.

Matereality Global Data Center
Matereality LLC, New York
http://www.matereality.com/

The Materials Global Data Center is a commercial data supplier. It provides over 160K tensile data sets, 40K stress-strain curves, and 7K viscosity results. The amount of ceramic data included is uncertain. The cost to access is $385/year.

JAHM Software
JAHM Software, Inc., Reading MA
http://www.jahm.com/index.html

This database provides access to over 2,600 materials and 22,000 sets of temperature-dependent data on elastic modulus, thermal expansion, thermal conductivity, electrical conductivity, specific heat, etc. There are a significant number of ceramic materials included in the database. There is a demo version, which includes data on the chemical elements. The cost to access the Materials Property Database (MPDB) depends on the number of licenses and currently runs from $350 to $595 for a perpetual access. There are no annual charges.

Material ConneXion Online Materials Database
Material ConneXion, New York, NY
http://www.materialconnecxion.com/

This site claims to contain the world's largest library for advanced materials. The coverage of ceramics properties is not clear. There is a fee to join and obtain any of their services. For example, an on-line subscription to their materials database is $250/year per individual. Academic pricing is also available.

ProQquest Deep Indexing: Materials Science
ProQuest, Cambridge Information Services, Ann Arbor MI
http://www.csa.com

CSA brings together the majority of the leading materials science databases, including ceramics and composites. Using its deep indexing technology, it can obtain charts and tables from within publications. It currently has over 4 million tables and figures on a variety of materials. Metadata are attached to each object. There are costs associated with each of its services.

Materials Properties Database
Makeitfrom
http://www.makeitfrom.com/

The data at this site were apparently taken from other sources, including "Ceramic and Glass Materials: Structure, Properties, and Processing," ed. by J.F. Shackelford and R. H. Doremus (2008). No test procedures or quality indicators are provided. Some data are free, but others require purchase of a temporary access.

Efunda
eFunda, Inc., Sunnyvale CA
http://www.efunda.com/materials/piezo/material_data/matdata_index.cfm

This database contains piezoelectric data on a number of materials, including barium titanate and PZT (lead zirconate titanate), as well as some semiconductors. Access is free.

B.7 Other Ceramics-related Data Resources

American Ceramic Society
http://ceramics.org

The American Ceramic Society provides access to a few data sources. It also maintains a database of ceramic producers.

ASM International
http://www.asminternational.org/

ASM is a professional society with extensive data activities. It does not have extensive ceramic data, but some ceramic property data are included in their Medical Materials Database.

Mindat.org
Mindat, Coulsdon, Surrey, England
http://mindat.org

Mindat.org is an online information resource that provides free mineralogical information. Data are obtained from voluntary submissions and are unevaluated. One can search by properties or chemistry.

Materials Digital Library Pathway (MatDL)
Kent State University, OH
http://matdl.org

The Materials Digital Library was created by a group of university and government researchers under the sponsorship of NSF. It does not have databases, but it does provide links to ceramic property data and graphs available at other locations.

Advanced Materials, Manufacturing, and Testing Information Analysis Center (AMMTIAC)
Alion Science, Rome NY
http://ammtiac.alionscience.com

AMMTIAC does not provide data *per se*, but it is the repository for large numbers of reports and publications. For example, if one searches on "ceramics," over 13,000 entries are returned. The staff can do searches for a fee. The site has links to other ceramics-related websites.

B.8 Ceramics-related Hard Copy Data Sources

Even though they are not available electronically, some important, high quality printed data sources should be included, as well, as listed below. While some are older references, their data are not yet available in electronic databases.

CRC Materials Science and Engineering Handbook
Ed. By J.F. Shackelford, W. Alexander, and J. S. Park
CRC Press, Boca Raton, Fla. (1994).

This book contains thermodynamic, physical, and mechanical property data for metals and ceramics. The data were extracted from other sources but do not appear to be evaluated.

Thermal and Other Properties of Refractories
Technical Report Program No. R056
Los Alamos Scientific Laboratory, Los Alamos, NM, (1973)

This report contains thermodynamic data (e.g., melting point, specific heat, enthalpy, crystal structure, density, thermal conductivity, thermal expansion, and hardness data) for a wide variety of ceramic compounds. References to the data are provided.

Single Crystal Elastic Constants and Calculated Aggregate Properties: A Handbook, 2nd Edition
Ed. by G. Simmons and H. Wang
MIT Press, Cambridge, MA. (1971)

This book is out of print but is extremely valuable, as it reports the elastic constant matrices for a very large collection of inorganic compounds. All of the data are referenced.

Elastic Moduli Data for Polycrystalline Oxide Ceramics
Ed. by R. G. Munro
NIST Internal Report 6853, Gaithersburg, MD (2002)

This report contains elastic property data for a variety of polycrystalline ceramics collected from the literature. Special attention is placed on the dependence of the moduli on porosity and temperature. For a number of the materials, an analytical model describing the simultaneous porosity and temperature data is provided.

Handbook of Optical Constants of Solids II
Ed. by E. D. Palik
Academic Press (1991)

This book contains critical reviews and tabulated values of indices of refraction and extinction coefficients for a large number of materials.

Data Evaluation Theory and Practice for Materials Properties: NIST Recommended Practice Guide 960-11
Ed. by R. G. Munro
NIST, Gaithersburg, MD (2003)

This NIST practice guide provides a theoretical foundation for data evaluation and gives practical examples.