A PERSPECTIVE ON MATERIALS DATABASES

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ABSTRACT

Several challenges are involved in developing and maintaining materials property databases, including improvements in measurement procedures, the changing nature of materials, access to proprietary data on new materials, and the need for quality evaluation. In this paper we discuss each of these issues and their impact on the availability of high quality material property data, using ceramics as an example material.

Keywords: Materials data, Ceramics data, Ceramics properties, Data quality, Materials databases

1 INTRODUCTION

It is widely accepted that convenient access to reliable materials property data is vital to the development of innovative components and devices. These data are necessary both for the design of new and complex multi-material structures and for the development of hitherto unknown materials as well as for new combinations of existing materials. Unfortunately, at this time, property data on new and emerging materials are either widely dispersed or entirely unavailable to the commercial, academic, and government research communities. Data that are available are frequently unevaluated or obtained through unknown or unreliable measurement procedures. Uncertainty regarding the accuracy of such data can be an impediment to its use.

In addition, modeling and theoretical calculations of properties are becoming more frequently employed instead of expensive and time-consuming physical measurement. One of the conclusions of a recent National Research Council report on Integrated Computational Materials Engineering (ICME) (National Research Council, 2008) is that databases are required for capturing, curating (culling and selecting), and archiving the critical information required for the development of the ICME area. The field of ceramics can be used as a prototype for the issues facing the development and maintenance of a materials property database in today's environment. For this paper, we defined ceramics as inorganic non-metals, e.g., semiconductor materials, glasses, as well as oxides, nitrides, carbides, and borides.

Today, almost all information, including factual property data, is generated, and can be collected, electronically. Key questions include: Do users want and need a single point of access for ceramics data? Are they willing to pay for it? What are the costs of maintaining such a resource? Keeping a data resource current is especially important because materials change over time, especially in the case of ceramics, where a variation in starting materials or processing conditions can make a significant difference in the properties of the final product. Users of ceramics databases demand up-to-date information, which can be difficult to provide.

Among the challenges involved in developing and maintaining materials property databases are a number of issues that are specific to the nature of materials, especially those used in commercial products. These issues include (1) improvements in measurement procedures, (2) lack of material specifications, (3) access to proprietary data on new materials, and (4) the need for quality evaluation. We discuss each of these issues in turn and their impact on the availability of high quality material property data, using ceramics as an example material.

2 IMPROVEMENTS IN MEASUREMENT PROCEDURES

Over the years, numerous test methods have been developed for engineering and other materials to help product designers understand the likely performance of a material in a specific application. This allows for testing of samples of potential materials to be done before a product is actually built. The materials and engineering communities have over time correlated the test results with actual service performance, thereby reducing over-design, facilitating substitution with a better or cheaper material, and providing direction for development of improved materials. In addition, over time the testing procedures are refined and codified in national and international standards test procedures.

As new testing procedures are developed, test data from previous decades may not stand up to today's scrutiny. As an example, a comprehensive database on the fracture toughness and crack growth characteristics of inorganic glasses was established at the National Institute of Standards and Technology (NIST - then the U.S. National Bureau of Standards) over twenty years ago (http://www.ceramics.nist.gov/srd/summary/advmatdb.htm). The database was created by collecting data from the literature. Quality evaluation was applied at the time, but today it is recognized that many of the test procedures used then have been improved upon or known to produce faulty results, so the test data are of little value today. This situation is not an isolated one.

3 THE CHANGING NATURE OF MATERIALS

In contrast to many other things found in nature, e.g., astronomical objects, crystals, etc., which do not vary over time, most materials are constantly changing, with respect to overall composition, surface finish, properties, and other factors. This is especially true for materials used in commercial products. Collecting data on permanent objects, such as a crystal, is relatively straightforward; with time, a complete collection of properties of the object can be created, even though measurements are made at different times and by different groups. In the case of materials, however, new materials are constantly being developed, while existing materials are changed, often in subtle ways, in composition and properties to improve performance or reduce cost. To make a data resource relevant, therefore, the resource must be refreshed and updated on a regular basis.

A particular problem with respect to ceramic property databases is a lack of rigorous specifications. The features of interest, e.g., microstructure, composition, purity, physical properties, that significantly affect properties may vary among different materials, even those with the same designation. A good illustration of this problem is aluminum oxide. The designation of a material as a 96% alumina means only that 96% of the bulk material is Al_2O_3. It says nothing about the other constituents, the processing procedures, or the properties. Every 96% alumina could be a different material with significantly different properties. Consequently, even though there are many test results for a wide variety of properties of 96% alumina, a user cannot be sure that the data are relevant to a specific use. Presently, even though advanced ceramics are potentially useful in many new applications, the lack of tight specifications limits their adoption, and unfortunately there is no coordinated effort to correct the situation. For other materials such as polymers and composites, the lack of good specifications causes the same problems.

4 ACCESS TO PROPRIETARY DATA ON NEW MATERIALS

Cost and performance competitiveness are always significant issues. In response, materials producers are continually redesigning, improving, and changing commercial materials. In many instances keeping proprietary data protected is critical for the economic success of the product or a company. Consequently, one can conclude that significant quantities of data on the newest materials and latest materials advancements as developed by commercial materials producers will be in large scale databases only after a significant time lag.

The result of this delay is that users of ceramics databases (and this also applies to all types of materials) are working with less than complete information while making decisions such as materials selection or performance prediction. This problem is exacerbated by the fact that for many materials classes, there are multiple producers and contacting all of them for their latest materials is an almost impossible task. So far the materials database community has not yet devised methods for at least alerting users that new materials with improved properties or performance might exist and that specific material producers should be contacted for further information.

5 THE NEED FOR QUALITY EVALUATION

Ceramic property data, and all material property data, can be obtained through internet search systems and scanning of reports and published literature. Important questions relate to the quality, reliability, and provenance of these data. For example, which test procedures were used to obtain the data and were they carried out in a proscribed manner? In most instances, the individual needing the data is not an expert on the testing procedures and therefore cannot properly place a value on the quality of the data obtained.

Are data useful even if their pedigree is uncertain? Are any data, despite uncertainty in their quality, better than no data at all? That is, must data be evaluated by experts to be useful or valuable? Evaluation is expensive. It is not clear who would carry out such a task, nor is it clear who would be able and willing to pay for comprehensive evaluation services. Is self-evaluation a way to avoid the high costs of experts in a particular materials field? A publication by Ronald Munro (2003) addresses such a question and provides a fundamental foundation for evaluation of material property data.

The International Centre for Diffraction Data (http://www.icdd.com/) makes available a "quality mark" option which allows the user to select only the most accurately determined patterns or to obtain all patterns regardless of quality. The "quality marks" reflect the type of X-ray diffractometer used, the degree of characterization of the chemical composition, an objective measurement of intensity, and the spread in the peak positions.

The assessment of data quality, similar to other quality issues, is a business decision. How much is the user, or his organization or company, willing to pay for high quality? Some of the most significant uses of materials property data are in the design and manufacture of components. The quality question becomes: How reliable are the material property data upon which we are basing design decisions? If we are not confident that we understand the uncertainty associated with a particular property value, are we willing to invest in making new and better measurements to reduce that uncertainty? Or are we willing to accept the property value and just over-design, thereby increasing the cost of the component?

Materials data are also needed for failure analysis, processing improvement, product improvement, and cost reduction. However, a significant consideration in investing in materials property data is its perceived value to the user. Routine uses of materials data may not be viewed as being worth the significant cost to develop, maintain, and update a database. Additionally the value of data is often forgotten after its immediate use, especially if the data are used early in a planning and design process. As a consequence, there is an unwillingness to pay the real value of accessibility to materials data. On the positive side, some long term investments have been made in collecting and providing access to materials data whose quality has been assessed that continue to provide value. Prime examples of these investments in data quality are phase diagrams and crystallographic data.

Ceramics Phase Diagrams

NIST has partnered with the American Ceramic Society (ACerS) for over 70 years in the collection, evaluation, and dissemination of ceramic phase diagrams (http://www.nist.gov/srd/nist31.htm). Systems include oxides, borides, nitrides, salts, and electronic ceramics. 22,000 evaluated diagrams plus commentaries are now available on CDs and in 21 bound volumes. An economic assessment study of the NIST-ACerS phase diagram program conducted in 1998 came to the conclusion that this program provided a benefit-to-cost ratio of approximately 10 to one.

Inorganic Crystallographic Database

NIST partners with FIZ Karlsruhe to provide needed crystallographic data on inorganic crystals (http://www.nist.gov/data/nist3.htm). The database currently contains 132,000 peer-reviewed data entries including atomic coordinates. NIST also provides a crystal database for both inorganic and organic materials and a structural database for metals and inter-metallic materials.

These databases contain high-quality, fundamental property data of materials, which remain of great value over decades. Performance property data, which is much more dependent on material composition and often varies over time as material composition changes, has not yet been successfully collected in long term programs in the same manner, especially with quality assessment in mind.

6 SOME TRENDS FOR THE FUTURE

With an increased use and development of nanomaterials has come an even greater need for sharing of critical materials property data. A new awareness of the importance of ready access to materials data and information has resulted in recent publications that discuss the current needs for materials informatics (Rogers & Cebon, eds., 2006). Most of the issues that apply to ceramics, including the funding and curating of databases, data mining techniques, linking databases to literature, and providing single point access, will be critical for nanomaterials as well.

One of the crucial areas of need for information exchange is that related to environmental, health, and safety issues posed by these new materials. Regardless of the problems, information technology brings new capability to materials data users. The Social and Semantic Webs continue to evolve rapidly as mechanisms for materials data access and exchange. Modeling, simulation, and knowledge discovery tools, as they become viable alternatives to materials testing, contribute new types of materials data, with different types of provenance and quality indicators. How that happens will be very interesting.

7 SUMMARY

The complexity of materials and the existence of disparate materials classes have complicated the development of large scale material property databases. While different sectors of the materials community have developed important data collections, the diversity and complexity of materials hinder strong business cases for the fully integrated materials data system envisioned nearly forty years ago.

Despite the acknowledged need for data and protestations regarding the lack of access, the costs of developing and maintaining a comprehensive modern data system are higher than any one entity, i.e., company or government agency, can afford. A primary question is whether methods exist by which such a system(s) can be created based on shared costs. An additional question is what is the minimum level of expertise and sophistication needed to create worthwhile systems?

The last thirty years have seen tremendous changes in the technology available to provide new types of access to materials data. The same time period has provided many lessons about meeting the challenges of digitizing, managing, and providing access to diverse types of materials data. Much of the progress made is the direct result of a robust planning process carried out in the 1980s that involved virtually every segment of the materials data community.

The time has come to plan for the future and not only assess where we are, but where we need to go. This assessment requires understanding of what and how material property data are currently available electronically on an international basis. The prioritized needs over the next decade for materials property data in government-funded research as well as by commercial material developers and manufacturers and academic researchers must be determined. It is critical to determine viable business models that can be applied to establish a sustainable materials property data access approach.

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