

# 98-3 Planning Report

## Economic Assessment of the NIST Ceramic Phase Diagram Program

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for

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# **ECONOMIC ASSESSMENT OF THE NIST CERAMIC PHASE DIAGRAM PROGRAM**

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Prepared for:

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Program Office  
Strategic Planning and Economic Analysis Group

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## **EXECUTIVE SUMMARY**

The National Institute of Standards and Technology (NIST) assists the ceramics industry by generating technical knowledge to improve the development and production of ceramic materials. The primary purpose of this case study is to assess the economic impacts on domestic industry for investments made in this infrastructure technology through the NIST Ceramic Phase Equilibria Program.

Phase equilibria relations are fundamental to the development and utilization of ceramic materials used in advanced applications. Temperature, pressure and material concentration are the principal variables that determine the kinds and amounts of phases (primarily, solid and liquid structures) present under equilibrium conditions. To ceramists, who must understand the effects of these variables on both the processing and the properties of finished ceramic products, phase diagrams provide the necessary information for phase equilibria relations. A phase diagram is a map indicating the areas of stability for various phase reactions as a function of external conditions.

The outputs from the NIST Program under examination are technical evaluations of phase equilibria diagrams. From these outputs, ceramic component suppliers derive two main types of benefits: (1) avoidance of duplicative R&D costs in the design of new ceramic materials, and (2) a means of explaining abnormalities that may arise in the production of ceramic materials. Phase diagrams are important especially to the suppliers of advanced ceramic materials. These suppliers serve a domestic market that is estimated at \$5.5 billion in 1995 and projected to grow by 9.5 percent per year to \$8.7 billion in 2000.

A hypothetical, counterfactual experiment has been used to evaluate the outcomes of the NIST Program outputs. The results show that, in lieu of NIST's investments, ceramic manufacturers collectively would be less efficient in attaining comparable technical data. Ceramists would incur greater costs for internal research and experimentation as well as delays in introducing innovative ceramic materials to market. Such economic inefficiencies would certainly have an adverse effect on the international competitiveness of U.S. ceramic component suppliers.

The internal rate of return (IRR) from investments in the NIST Phase Equilibria Program has been calculated to be at least 33.5 percent. This calculation is based on a five-year appraisal of prospective economic benefits and expenditure data related to the outputs of the NIST Program. Net benefits have been estimated from a survey of the domestic advanced structural ceramics

industry using the hypothetical, counterfactual experiment. A number of factors have been incorporated to portray this as a conservative estimate of NIST's economic impact on domestic industry. Using a similar set of factors and assumptions, the benefit-to-cost ratio (BCR) is 10.0 to one. The conservative estimates of the IRR and BCR imply that the NIST Phase Equilibria Program is pursuing a socially-valuable activity affecting the domestic ceramics industry and a larger range of downstream industries.



# 1.

## INTRODUCTION

### 1.1 NIST

The United States Department of Commerce (US DoC) through the National Institute of Standards and Technology (NIST) supports U.S. industry's efforts to develop new technologies, accelerate commercialization of new products and processes based on these technologies, and achieve global market penetration to advance the Nation's economic growth and standard of living. NIST's laboratories provide this support in the form of various types of nonproduct standards, testing, and laboratory accreditation services that are used by industry in meeting the challenge of keeping pace with rapid technological change. NIST is the only Federal laboratory with the primary mission of supporting the development and commercial application of technology.

NIST's laboratories develop and transfer infrastructure technologies to industry. Infrastructure technologies (infratechnologies) are "tools" that make the R&D, production, and market penetration stages of the product cycle more efficient. These tools enable industry to efficiently develop applications that are based on both generic and proprietary technologies.<sup>1</sup> Examples of infratechnology tools include production methods, processing models, advanced measurement methods, technical databases, nonproduct standards, product performance tests, and quality assurance techniques. NIST develops its tools commensurate with the commercialization needs of U.S. industry, which have become ever more demanding.

### 1.2 MATERIALS SCIENCE AND ENGINEERING LABORATORY

The NIST Materials Science and Engineering Laboratory (MSEL) provides technical leadership and participates in developing the measurement infrastructure related to materials critical to U.S. industry, academia, government and the public. The overall mission of MSEL is to foster the development and processing of safe and efficient products by improving the quality, manufacturability, and reliability of these materials. This mission is accomplished through developing and disseminating nonproduct standards, measurement methods, predictive models, evaluated data and reference materials, and the scientific, quantitative understanding that is fundamental to the synthesis, processing, characterization, properties, and performance of materials. Materials science and engineering programs at NIST cover a full range of materials issues from design to processing to performance.

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<sup>1</sup> The role of infrastructure technology within the construct of product development is discussed in: Gregory Tassey, *The Economics of R&D Policy*, (Quorum Books, 1997; Chapter 8); and Albert N. Link and Gregory Tassey, *Strategies for Technology-based Competition*, (Lexington Books), pp. 16-21, 1987.

The NIST/MSEL Data Technologies Program develops and facilitates the use of evaluated databases for the materials science and engineering communities. Both research- and application-directed organizations require readily-available, evaluated data to take advantage of the large volume of materials information developed in public- and private-sponsored programs. This information, particularly numeric data, is available in an ever increasing number of worldwide publications. The necessity to consolidate and allow rapid comparison of materials properties for product design and process development underlies the database projects performed within NIST. These projects are conducted in cooperation with the NIST Standard Reference Data Program Office, and include compilation and evaluation of numeric data as well as recent efforts directed at more effective distribution and use of the data.<sup>2</sup>

### **1.3 NIST/ACerS PHASE EQUILIBRIA PROGRAM**

#### **1.3.1 History, Purpose, and Objectives**

More than a 100 years ago, scientists discovered the usefulness of phase diagrams for describing the interactions of inorganic materials in a given system. Phase equilibria diagrams are graphical representations of the thermodynamic relations pertaining to the compositions of materials. Ceramists have long been leaders in the development and use of phase equilibria diagrams as primary tools for describing, developing, specifying and applying new ceramic materials. (For a more detailed description of ceramic phase equilibria diagrams, see Appendix A).

For over 60 years, NIST and The American Ceramic Society (ACerS) have collaborated in the collection, evaluation, organization and republication of phase diagrams for ceramists.<sup>3</sup> During that time, over 10,000 diagrams have been published by ACerS through its close working relationship with NIST. The collaboration between these two organizations was informal until December of 1982, and successive formal agreements have extended the program to the present time.

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<sup>2</sup> The 90th Congress passed PL 90-396, HR 6279 on July 11, 1968 identifying NIST as the responsible organization for providing the collection, compilation, critical evaluation, publication and sale of standard reference data.

<sup>3</sup> This collaboration began in the late 1920's and early 1930's between Herbert Insley of the National Bureau of Standards (NIST's organizational name prior to 1988) and F.P. Hall of Pass and Seymour, Inc. (Syracuse, New York). Their initial monograph "A Compilation of Phase-Rule Diagrams of Interest to the Ceramist and Silicate Technologist" was published in the October 1933 issue of the *Journal of the American Ceramics Society*, ACerS' main technical journal.

The purpose of this program, known generally as the Phase Equilibria Program, is to support growth and progress in ceramics industries by providing qualified, critically-evaluated data on thousands of chemical systems relevant to ceramic materials research and engineering.<sup>4</sup> This information serves as an objective reference for important statistical parameters such as melting points and chemical reactivity. In short, the database is a valuable source of infrastructure technology for ceramists in research- and application-oriented organizations.

The intention of the Program is to overcome problems that researchers have in using ceramic phase equilibria diagrams that appear in the various technical journals. For example, the original source of a diagram is often obscure or not available readily to all ceramists. Diagrams are also published with inconsistent styles and units, and some diagrams are published with obvious (to expert ceramists) errors in thermodynamic data which result in design failures. Maintaining currency (the constant updating of diagrams) is another concern of ceramists. Hence, the objective and scope of the NIST/ACerS program is to compile an accessible, accurate, systematic, and current set of phase diagrams that have already appeared in the archival literature.

The Phase Equilibria Program benefits the industrial community of ceramists in a number of ways. The use of accurate, evaluated phase diagrams — versus incorrect diagrams — minimizes design failure, overdesign, and inefficient processing. Another impact is the reduction in duplicative research performed by individual ceramists. The savings in time and resources to search and evaluate the phase diagrams individually can be directed more productively to applied research on the material of interest. Also, the ready access of qualified diagrams can spur the insertion of ceramic materials into new applications. For example, the availability of high-quality diagrams is credited with the rapid development of ceramic materials used in the cement and metals processing industries.

The primary output of the NIST/ACerS Phase Equilibria Program has been the compilation of evaluated data. These data have been published as *Phase Diagrams for Ceramists (PDFC)*, mostly in printed form but also in electronic form in recent years. The current set of PDFC consists of 14 major volumes and 11 smaller compilations, and each PDFC document encompasses a particular niche of ceramics. ACerS estimates that over 45,000 individual copies of the 14-volume set have been sold since 1933.

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<sup>4</sup> Richard M. Spriggs and Stephen W. Freiman, “ACerS/NIST Phase Equilibria Update,” *The American Ceramic Society Bulletin*, Volume 75, No. 1 January 1996.

### 1.3.2 Management

The Phase Equilibria Program is managed under the Phase Equilibria Program Committee of ACerS. Committee membership includes Society members, the ACerS Executive Director and the Chief of the Ceramics Division of NIST/MSEL. Other Society and NIST employees serve as important resources to the Committee. Selection of diagrams from the available technical literature is one of the tasks of this Committee. The diagrams selected for evaluation and compilation are meant to: meet the pressing needs of researchers, students and industry; have economic importance; and promote advanced technology.

Under the current joint arrangement, NIST administers the technical aspects of the Program and ACerS oversees the publication of data. Organizationally within NIST, the Phase Equilibrium Program is a project within the Data Technology Program described in Section 1.2, above. NIST provides overall coordination and technical guidance, ensures quality data coverage and evaluation with expert commentary, and develops the prototype software configurations of the phase diagrams.<sup>5</sup> Oftentimes, the actual evaluation is performed by reviewers from academia, industry and government laboratories outside of NIST as well as by consultants. ACerS is responsible for preparing, disseminating and operating database outputs in electronic and printed forms. These responsibilities are carried out through full-time research assistantships at NIST.

The Phase Equilibria Program is funded by a combination of sources. ACerS contributions come from a mix of endowment income and net proceeds from sales of PDFC volumes. NIST provides funding from the NIST/MSEL Standard Reference Data Program and the Ceramics Division. Table 1 shows annual expenditure data for NIST from 1985 to 1996.<sup>6</sup> NIST's research efforts during this time have been incorporated in nine PDFC volumes, six of which pertain to advanced ceramics.

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<sup>5</sup> NIST personnel in the Ceramics Division conduct research on the development of new phase diagrams, but this research is not within the scope of the NIST/ACerS Phase Equilibria Program.

<sup>6</sup> This expenditure data was obtained from personnel in the NIST/MSEL Ceramics Division. NIST's expenditures include (1) direct, fully-burdened labor of laboratory personnel, and (2) consultants/subcontractors. Operating funds from other government agencies are negligible.

**Table 1 NIST Phase Equilibria Program Research Expenditures (\$000), 1985-96**

Year	NIST Research Expenditures
1985	420
1986	420
1987	382
1988	294
1989	255
1990	265
1991	87
1992	94
1993	103
1994	105
1995	97
1996	136

#### **1.4 CASE STUDY OBJECTIVES**

This case study provides an estimate of the first-order economic impacts on U.S. industry from NIST's contribution to the NIST/ACerS Phase Equilibria Program. NIST's infrastructural outputs are examined in terms of the affected industrial activities, the qualitative nature of the impacts on the behavior of relevant industries, and the quantitative impacts on the competitive performance of these industries. The specific objectives established at the onset of the study were to :

- Describe the practical use and economic importance to ceramists of phase diagrams and the corresponding infrastructure technology developed by NIST
- Analyze the affected industry structure and marketing strategies
- Characterize technical barriers encountered by industry which have been addressed by NIST via the development of infrastructure technology
- Obtain qualitative and quantitative data on the economic impacts attributable to the infrastructural outputs from NIST; these economic impacts include assessments of the benefits and costs from the perspectives of users, producers, and other organizations that influence and are influenced by products made with ceramic materials
- Analyze the data and calculate the rate of return on NIST's investments in this infratechnology using various economic measures

- Prepare a report of the findings, analyses and conclusions

## **1.5 CASE STUDY OUTLINE**

The remainder of this report includes the following:

- Chapter 2 describes both the role of ceramic phase diagrams in industrial applications, and the domestic advanced ceramics industry which is the segment of the broader ceramics industry under focus in this case study
- Chapter 3 describes the scope, benefit measures and data collection strategy used for the analysis in this case study
- Chapter 4 identifies findings on the qualitative and quantitative economic impacts of the infrastructural outputs from the NIST Phase Equilibria Program based on a survey of advanced structural ceramic producers
- Chapter 5 provides quantitative estimates of the prospective economic rate of return from investments made in the NIST Phase Equilibria Program
- Chapter 6 discusses the primary conclusions for this case study
- Appendix A provides a technical overview of ceramic phase diagrams

## 2.

## BACKGROUND

### 2.1 ROLE OF PHASE DIAGRAMS IN INDUSTRIAL APPLICATIONS<sup>7</sup>

The evaluation and availability of phase diagrams are extremely important for the economic well-being of the ceramic industry. In the past, industry representatives have estimated that the lack of readily available compilations of evaluated phase diagrams costs industry many millions of dollars per year due to:

- Product failures resulting from materials based on unreliable thermodynamic data
- Unnecessary overdesign and waste
- Inefficient materials processing
- Needless duplication of research and development which occurs when the data sought have already been generated but published in obscure journals

The remainder of this section provides examples of the importance to ceramists of phase diagrams and the NIST/ACerS Phase Equilibria Program.

The manufacture of refractories (ceramic materials that are resistant to melting at high temperature) depend on accessible and accurate phase diagrams. Figure 1 shows a phase diagram of silicon dioxide and aluminum oxide. This particular diagram is significant to the ceramics industry because many refractories are made from combinations of these common materials. Figure 2 shows an industrial example, a burner port block, which was composed of a 65 percent aluminum oxide refractory, degraded and deformed in a gas-fired furnace after only a few months of use. The operating temperature in the block was found to exceed 1,595 degrees Celsius (°C). As the phase diagram indicates, a certain amount of liquid phase develops in this material which explains the easy deformation of this refractory. By using a material with higher alumina content, that is, between 70 and 80 percent, only solid phases exist at temperatures around 1,600 °C. Such material is more stable against deformation and degradation and has a longer useful lifetime. This is a prime example of how phase diagrams have been used in the design of ceramic applications.

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<sup>7</sup> This section is based mainly on excerpts from the unpublished manuscript by Dick Spriggs, "ACerS Phase Diagram Program," July 1988.

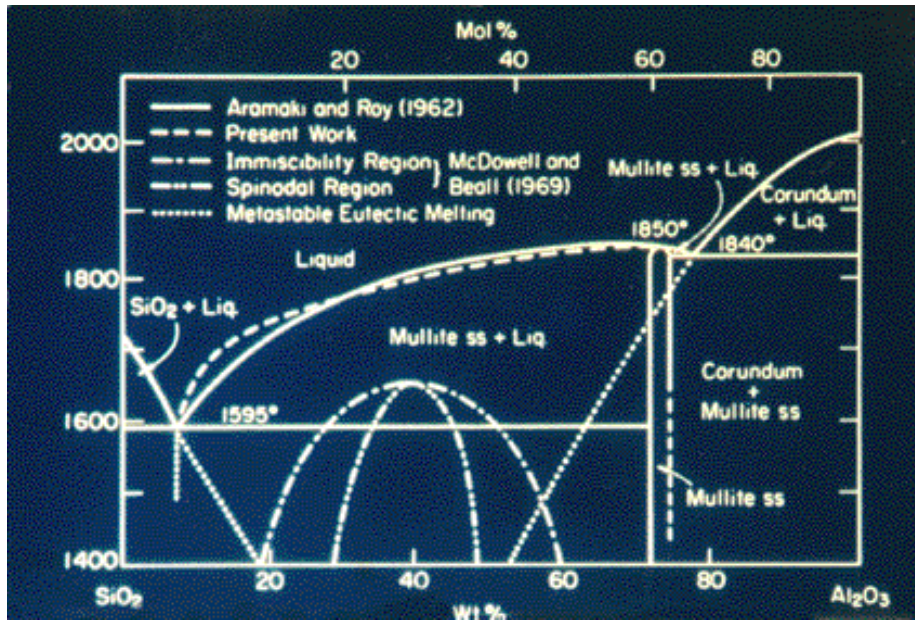


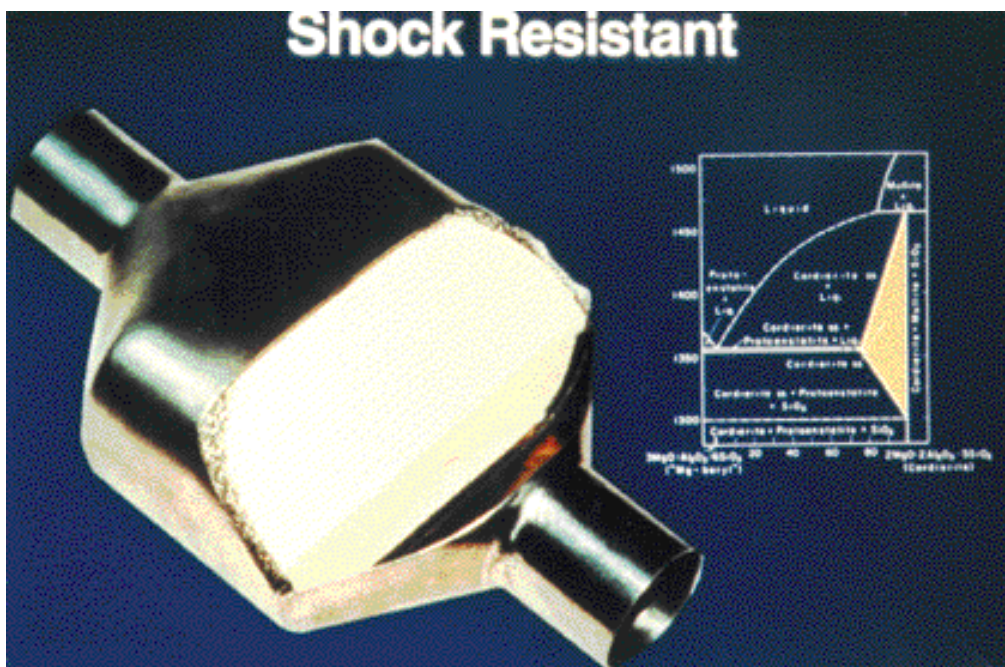
Figure 1 SiO<sub>2</sub> - Al<sub>2</sub>O<sub>3</sub> System



Figure 2 Burner Port Block Application



Another example of the impact of phase equilibria is the catalytic converter used for automotive emission control. In the center of the catalytic converter, shown in Figure 3, is the ceramic catalyst support produced by Corning, Incorporated. This honeycomb material is frequently made from a magnesium aluminum silicate (shown in the highlighted portion of the phase diagram) because of its characteristics for low thermal expansion and high use temperature. Manufacturing is difficult because, as the figure indicates, this material has a steep liquid-solid curve whereby only small changes in composition produce an excess of the liquid phase. To manage these physical changes, the firing temperature and processing composition of this material must be controlled accurately. This control requires a very accurate phase diagram in the vicinity of the desired composition.



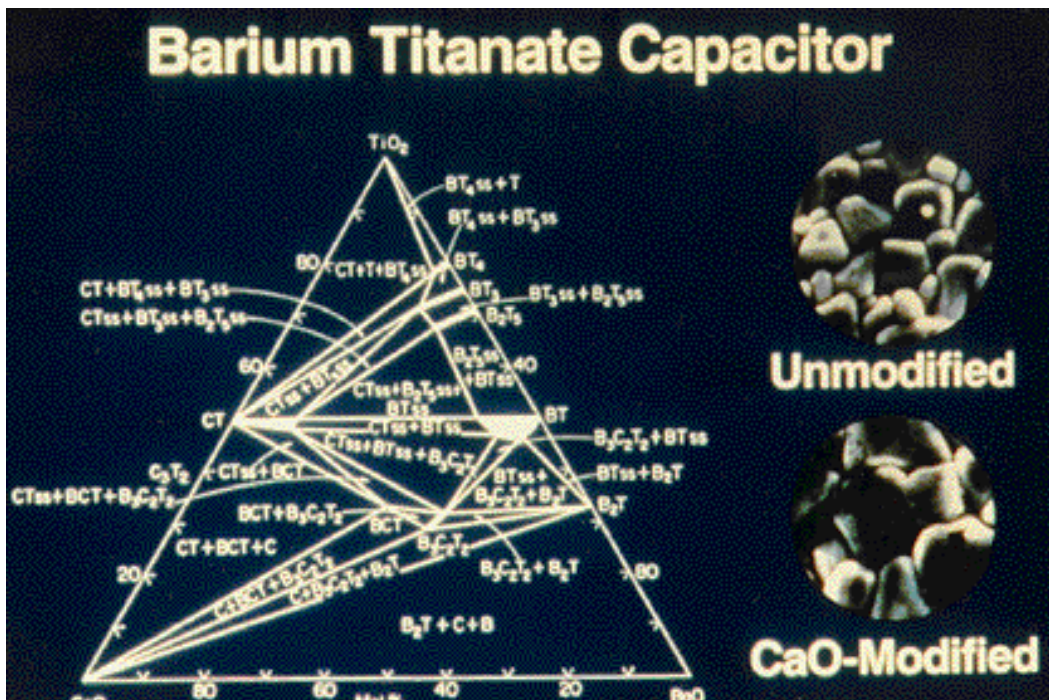
**Figure 3 Catalytic Converter Application**

In fact, the PDFC volumes played a critical role in establishing this product technology into an important business for Corning. Accurate phase diagrams were essential for developing the most durable material composition. Corning estimates that the ceramic catalyst support has now been installed in 500 million automobiles and small trucks world-wide, and this product has played a major role in reducing environmental pollution.

Phase diagrams are especially important to manufacturing new ceramic products, such as the ceramic fibers and coatings made from combinations of silica and boria which have been developed with sol-gel process technology. In these processes, the ceramic materials are made from two very different

precursor materials. The sophisticated products made from ceramic materials, such as the thermal insulation used on NASA's Space Shuttle, continue to provide solutions for practical engineering problems.

Accurate phase diagrams are also important in the area of electronic ceramics. The titanium oxide, calcium oxide, barium oxide phase diagram shown in Figure 4 includes the most common material, barium titanate, used for ceramic capacitors. The complex phase diagram shows that small additions of calcium oxide have large effects on the phase composition and the physical parameters of the capacitor material. Therefore, accurate phase diagram information allows developers to understand the changes occurring in materials properties, and, in turn, to better understand capacitor performance.



**Figure 4 Barium Titanate Capacitor Application**

Electronic ceramic capacitors are also produced from combinations of barium oxide and  $\text{TiO}_2$ . Using Figure 5, efforts to develop a temperature-stable capacitor based on the compound at 80 percent  $\text{TiO}_2$  ignored the compound to the right because it did not exist in the old phase diagram literature. But subsequent investigations into the phase fields of higher  $\text{TiO}_2$  content produced the superior material required for temperature-insensitive capacitor materials. This work has proved important to the market for reliable, temperature-stable electronics for satellite communications. AT&T Bell Laboratories credits the availability of an accurate and improved phase diagram in obtaining a patent on this material which provided AT&T with a competitive advantage in developing reliable satellite systems.



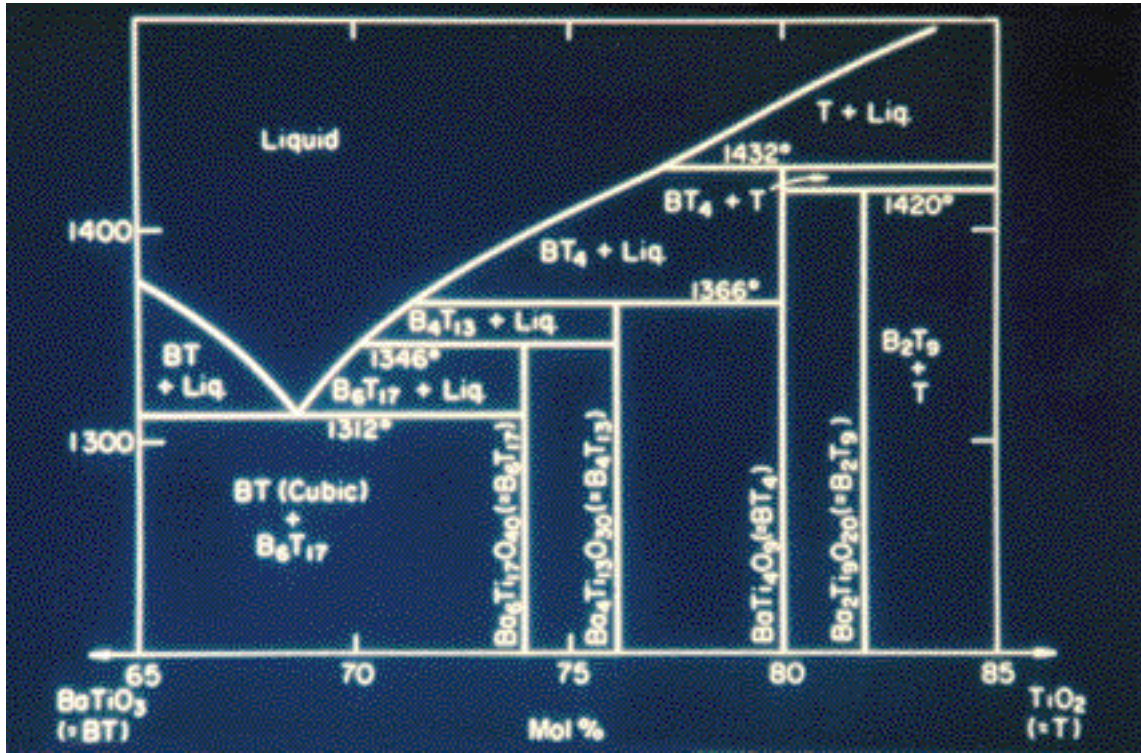
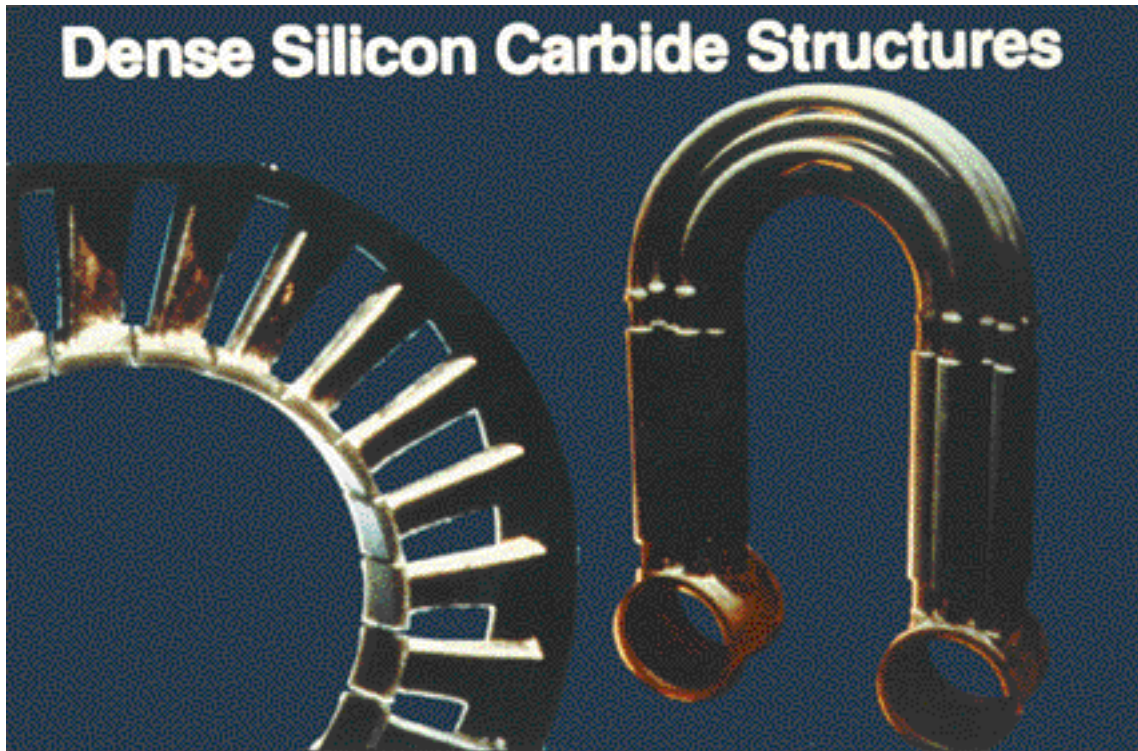


Figure 5 BaTiO<sub>3</sub> – TiO<sub>2</sub> System

Silicon carbide and silicon nitride are the primary materials for a market in advanced ceramic materials estimated to total \$20 billion during the next 15 years. Figure 6 shows two examples of dense silicon carbide in the complex shapes needed for these future technologies. The part on the left is a stator (a stationary component enclosing rotating parts) for an automotive gas turbine engine and the large structure on the right is a section of a ceramic heat exchanger tube array. Accurate phase diagrams are extremely important for fabricating these new, high-technology materials. Furthermore, accurate phase diagrams of these materials in combinations with oxides and combustion gases will be important for understanding their performance in the potentially corrosive environments that they are designed to endure.



**Figure 6 Complex Silicon Carbide Structures**

## **2.2 INDUSTRY AND MARKET FOR ADVANCED CERAMICS**

Ceramic materials are divided into two general categories: traditional and advanced. Traditional ceramics include clay-base materials such as brick, tile, sanitary ware, dinnerware, clay pipe, electrical porcelain, common-usage glass, cement, furnace refractories and abrasives. Advanced ceramics are often cited as enabling technologies for advanced applications in fields such as aerospace, automotive, and electronics.

Advanced ceramic materials constitute an emerging technology with a very broad base of current and potential applications and an ever growing list of material compositions. Advanced ceramics are tailored to have premium properties through application of advanced materials science and technology to control composition and internal structure. Examples are silicon nitride, silicon carbide, toughened zirconia, aluminum nitride, carbon-fiber-reinforced glass ceramic, and high-temperature superconductors. This section describes the domestic industry and market for advanced ceramic materials, and, in particular the structural segment of this industry, which is the focus of the industrial survey for this case study.

### **2.2.1 Industry Structure**

According to Business Communications Company (BCC), a market research firm that follows the advanced ceramics industry, over 450 U.S. companies (including foreign-owned subsidiaries) are involved in the business of advanced ceramics. Of this total, approximately 125 firms produce structural ceramics. Firm size ranges from the job shop to huge multinational corporations, and considerable variation also exists among individual firms regarding their degree of manufacturing integration.<sup>8</sup>

Current trends in this industry are for greater emphasis on the systems approach for the commercialization of new products. The systems approach comprises the full spectrum of activities necessary to produce the final system or subsystem, including production of raw materials, product design, manufacturing technology, component production, integration into the subsystem or system design and final assembly.

The systems approach has resulted in new corporate relationships in the advanced ceramic industry. More consolidation of efforts between companies is occurring due to the following factors: complex technical requirements; the level of sophistication necessary to manufacture advanced ceramics; the advantages in pooling technology, personnel and/or company facilities; and the finite amount of business that can support these suppliers. Indications of this consolidation are the 180 acquisitions, mergers, joint ventures and licensing arrangements identified by BCC from 1981 to 1995 for firms in the advanced ceramics business.

Research and developmental activities are carried out typically by large companies and institutions. However, a number of small start-up companies also attempt to commercialize products.

### **2.2.2 Markets**

Based on estimates from BCC, Table 2 summarizes the market size for the various advanced ceramic market segments in the United States. The total market value of U.S. advanced ceramic components for 1995 is estimated to be \$5.5 billion, and the year 2000 market is forecast to be \$8.7 billion for an average annual growth rate of 9.5 percent. Electronic ceramics has the largest share (about 75 percent) of this market in terms of sales, although the structural ceramics market is expected to have the largest growth rate in terms of massive use.

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<sup>8</sup> Thomas Abraham, "U.S. Advanced Ceramics Market Growth Continues," Ceramic Industry, October 1996.

**Table 2 U.S. Markets For Advanced Ceramic Components From 1995-2000**

	<b>1995 (\$M)</b>	<b>2000 (\$M)</b>	<b>AAGR 1995-2000 (%)</b>
Structural Ceramics	500	800	9.9
Electronic Ceramics	4,215	6,573	9.3
Environmental/Industrial	240	400	10.8
Ceramic Coatings	575	940	10.2
<b>Total</b>	<b>5,530</b>	<b>8,713</b>	<b>9.5</b>

AAGR - Average Annual Growth Rate

Note: All dollar values are in current U.S. dollars

Source: BCC

The market for U.S. advanced structural ceramics is expected to grow from \$500 million in 1995 to \$800 million in 2000 with a growth rate of 9.9 percent. Such materials are used for high-performance applications in which a combination of properties such as wear resistance, hardness, stiffness, corrosion resistance and low density are important. Major market segments are cutting tools, wear parts, heat engines, energy and high-temperature applications, bioceramics, and aerospace and defense-related applications. The largest market share is for wear-resistant parts such as bearings, mechanical seals and valves, dies, guides and pulleys, liners, grinding media, and nozzles.

While the market for advanced ceramics is expected to grow significantly into the next century, certain technical and economic issues have to be resolved to realize this potential. Such issues include high cost, brittleness, need for increased reliability, repeatable production of flawless components and stringent processing requirements for pure and fine starting powders with tailored size distribution. The advanced ceramic market, and in particular the structural ceramics market, could grow even further if these problems can be overcome by industry. U.S. government agencies, including NIST, will continue to have significant roles in resolving these problems to assist U.S. companies in achieving early commercialization of innovative ceramic technologies developed in this country.

### **3. EVALUATION FRAMEWORK AND APPROACH**

#### **3.1 SCOPE**

At the onset of the study, the TASC study team both reviewed the available literature and held discussions with NIST technical personnel and industry representatives. The main purpose of this fact-finding exercise was to understand the general use of phase diagrams in industry for determining the scope of the economic impact analysis. This exercise provided several pertinent, generalized facts:

- Phase diagrams are used primarily by ceramic component manufacturers, not at all by the suppliers of raw materials, and somewhat by systems manufacturers (generally, the customers of the component manufacturers)
- Available phase data obviate the need for industrial firms to gather these data separately, for which they may not have the required internal resources (time, equipment and expertise)
- The primary benefits of evaluated phase diagrams in the PDFC volumes are avoidance of R&D costs in the development of new ceramic materials, and, to a lesser extent, explaining abnormalities that may arise in the production of ceramic materials
- The legacy diagrams published many years ago by ACerS continue to have significant usage by industrial ceramists (verified by an ACerS' staff member who stated that Volume 1 of PDFC is still their best-seller)
- Ceramists in the four major market segments of advanced ceramic materials differ in their reliance on phase diagrams for product development activities; the order of reliance is as follows: structural, electronics, environmental, and coatings
- When necessary, ceramists readily use non-evaluated phase diagrams that do not appear in the PDFC volumes
- Standards do not apply to ceramic phase diagrams, and, typically, systems manufacturers do not specify particular phase diagrams in procurements with their suppliers of ceramic components

Using this information, the study team decided that the advanced structural ceramics industry would be the focus for collecting benefit data. Firms in this industry group use phase diagrams from PDFC volumes that were generated from a relatively recent period (since 1985). As such, these particular volumes became the outputs to be evaluated for economic impact. While industry realizes significant benefits from the earlier volumes, difficulties in obtaining credible cost data attributable to these outputs — from as far back as the 1930s — led to the decision of not quantifying benefits for such outputs.

Obviously, NIST's research efforts for the outputs under consideration diffuse beyond the target benefit group, the advanced structural ceramics industry. The downstream systems manufacturers benefit from performance improvements in ceramic componentry based on the know-how from the phase diagrams. Also, from a horizontal industrial perspective, the other segments of the advanced ceramic industry benefit in ways similar to firms in the structural ceramic industry. However, due to limitations of time and budgets for the study, the structural ceramics industry was determined to be an appropriate population for assessing benefits. Limiting the study scope to this population provides a basis for a lower bound estimate of industry benefits.

### **3.2 METHODOLOGY FOR ESTIMATING ECONOMIC BENEFITS**

The approach for evaluating the economic benefits associated with NIST's research outputs has been adopted from evaluations of other public investments in infratechnology.<sup>9</sup> Specifically, research costs are compared to an estimate of the benefits received by industry using a hypothetical, counterfactual experiment. The hypothesis for this experiment is that industry would have incurred additional costs in the absence of the NIST-conducted research. In other words, these are costs avoided by industry due to the existence of the NIST-conducted research and its availability through the PDFC volumes.

The counterfactual experiment is used because this case study lacks comparable baseline observations. Based on initial interviews with industry representatives, all firms in the advanced ceramics industry, broadly defined, appear to rely mainly on evaluated phase diagrams emanating from research conducted at NIST. If some firms relied on phase diagrams from alternative sources, then the production-related efficiencies between the two groups of industrial firms could be compared to ascertain a first-order measure of the added value attributable to the NIST-conducted research. Historically, all manufacturers in the industry appear to have access to the PDFC volumes and have had such access for years. Stated alternatively, the development and manufacture of structural ceramic materials and products has taken place in an environment based primarily on evaluated phase diagrams from NIST.

### **3.3 STRATEGY FOR COLLECTING BENEFIT DATA**

Previous experience in gathering information related to economic benefits associated with NIST's research programs suggests that the most efficient means of collecting benefit data is through semi-

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<sup>9</sup> See Tasse, 1997; Albert N. Link, *Evaluating Public Sector Research and Development*, (Praeger: New York, 1996); and Gregory Tasse, *Rates of Return from Investments in Technology Infrastructure*, NIST Planning Report 96-3, June 1996.



structured, interactive telephone interviews. Hence, that mode of data collection was chosen for this case study.

A telephone interview guide was prepared and pre-tested with several industry representatives, and later formally approved for data collection by the Office of Management and Budget. In summary, this interview guide was designed to elicit the following information:

- Examples in which the PDFC volumes were important in the commercialization of advanced ceramic products
- Likely action(s) that would have been taken if the appropriate phase data had not been found in the PDFC volumes
- Estimate of the economic impact from solving technical problems in lieu of the available PDFC volumes
- With respect to the use of phase diagrams, an estimate of how representative the example applications are compared to the firms' total commercialized products
- The frequency of use and handling of non-evaluated phase diagrams

Based on input from BCC and NIST, a sample size of 32 advanced structural ceramics firms was identified for contact. This group is representative of the broader population of manufacturers of structural ceramics products that directly utilize, through the PDFC volumes, NIST's evaluation research. According to BCC, these 32 companies represent about 60 to 70 percent of the domestic structural ceramics industry as measured in terms of annual sales.

NIST and ACerS identified a contact individual for each of the 32 companies. Each individual was initially contacted by NIST in order to:

- Briefly describe the purpose of the evaluation study as part of a NIST internal planning process
- Solicit their participation in a survey designed to identify economic benefits associated with the technical information in the PDFC volumes
- Introduce the TASC study team
- Assure each participant that individual survey responses would be kept confidential by the TASC team and only aggregate information would be provided to NIST for planning purposes

## 4.

## SURVEY RESULTS

Twenty-eight of the 32 representatives in the industry sample were interviewed by telephone. These 28 companies are listed in Table 3.

**Table 3 Participating Companies in the Telephone Survey**

• Advanced Cerametrics	• Engineered Ceramics
• Allied-Signal	• ESK Engineered Ceramics
• AISiMag Technical Ceramics	• Ferro Corporation
• APC International	• Greenleaf Technical Ceramics
• A.P. Green Refractories	• Ispen Ceramics
• Blasch Precision Ceramics	• Kennametal
• Ceradyne	• Lucent Technologies
• Ceramatec	• Norton
• Ceramco	• PPG
• Corning	• 3M
• Delphi Energy and Engine Management System	• Textron
• Dow	• Vesuvius
• Du-Co Ceramics	• WESGO
• DuPont	• Zircoa

### 4.1 QUALITATIVE OBSERVATIONS

#### 4.1.1 Summary Results

About half of the respondents followed the interview guide in a methodical fashion while the other half preferred to discuss the role of evaluated phase diagrams in a more unstructured manner. This mix in response styles created difficulty in characterizing the qualitative observations of the survey statistically. In lieu of a statistical analysis, several stylized facts on the general use of phase diagrams in the structural ceramic industry are described as follows:

- Phase diagrams are used most frequently during the research stage of the product cycle; product design/development was the next stage mentioned most frequently for the use of phase diagrams.
- When queried about the examples mentioned during the interview as to what action(s) would have been taken if appropriate evaluated phase diagrams were not available in the PDFC volumes, the responses were varied, but, two options were mentioned consistently:
  - (i) Search for non-evaluated equilibria data from other sources/publications, or

- (ii) Perform internal experimentation to determine the appropriate phase relations. In only one case did a respondent note a situation where a research project was halted.
- Regarding the perceived economic consequences associated with alternatives to the evaluated phase diagrams in the PDFC volumes, respondents were of the opinion uniformly that both certainty associated with the performance of the final product would decrease and the research or product design/development stage would lengthen by about six months (the median response).
- While ceramic researchers generally have greater confidence in evaluated diagrams in comparison to non-evaluated diagrams, they scrutinize all phase diagrams carefully in the area of the diagram of interest — whether it is an evaluated diagram or a non-evaluated diagram.

#### **4.1.2 Examples of Using the PDFC Volumes**

The survey respondents provided various examples of the practical use and economic importance of evaluated phase diagrams during the research or design/development stages of product development. Most of these examples were developed and commercialized many years ago — most going back to the 1970s — as most the respondents were reluctant to describe ceramic products developed and produced within the past five years, as requested. Hence, many of the examples technically are not considered advanced structural ceramics. Several testimonials from the interviews are paraphrased below to illustrate the breadth of applications and the importance of the PDFC data in product development.

- A respondent from 3M:

Our products are typically derived from knowledge of chemical solutions rather than melting points (melts). Products made from solution are superior to products made from melts due to the presence of far less contamination, although products developed with the former method are more expensive. The phase diagrams allow us to determine the appropriate material properties from a chemical solution.

For example, the PDFC diagrams have helped in the development of a product family of abrasive materials produced from solutions rather than melts. These materials are used to make sandpaper and grinding wheels. The research on abrasives began in 1971, the first product was introduced by 1980, and we've continued to develop it. Our first product was developed with magnesium oxide, and subsequent products have been made with aluminum oxide modified with various elements. We manufacture abrasives in the tons per day which is converted into miles of sandpaper. Our abrasive product line has been reformulated extensively in the last five years, all with the use of the PDFC volumes; overall, about 60 percent of our ceramics product line uses the PDFC data. In lieu of the evaluated NIST data, we

would perform (1) internal experimentation to determine the appropriate phase relations, or (2) "Edisonian" development or design of experiments without phase relation data.

Another example of our solution-derived materials is a zirconia silica fiber used for high temperature insulation and metal-matrix composites. These materials are used typically in aerospace applications such as the tiles, insulation, door seals and much more for NASA's Space Shuttle. We make hundreds of pounds a day of this material.

- A respondent from APC International:

In our business, we develop and sell products made from lead zirconate titanate, a transducer material that can change electrical energy to mechanical energy and vice versa. These ceramic products are used in ultrasonic-based applications (e.g., sonar, medical, flow and level control, and non-destructive testing and evaluation of materials). Our products are also found in diverse end-products such as ultrasonic cleaning equipment, welding equipment and chiming devices (e.g., the buzzer that rings for the seat belt in a car, or the ringer that signals that a washing machine has finished its cycle).

Essentially, one phase diagram in the PDFC is pertinent to our work in lead zirconate titanate products. A sensor material developed recently illustrates the use of this phase diagram. This material can be used to measure liquid flow through pipes, and it needs to have certain electrical properties and efficiencies in the transferring of mechanical to electrical energy. We began research on this product about three years ago, and the relevant PDFC diagram was important in understanding the structural phase boundaries in different situations. The product was commercialized about one year ago.

Similarly, the rest of our lead zirconate titanate product line refers to the PDFC data. Without the availability of the PDFC diagram we would have had to incur additional in-house research costs for experimentation to generate the relevant phase diagram, and the commercialization of our material would have been delayed at least six months and maybe as long as two years.

- A respondent from Dow Chemical:

Our company produces tungsten carbide powder materials which involves an understanding of recent phase diagrams. To illustrate, we developed three powders having very fine sizes: 0.2, 0.4, and 0.8 microns. These materials are intended for new applications (e.g., high speed drills for circuit board manufacturing) requiring very high strength. The phase diagrams helped us learn how to process the tungsten carbide powder. In the absence of the PDFC volumes we would have searched for non-evaluated phase diagrams rather than generate them ourselves. We would work with these non-

evaluated diagrams knowing that they may be less accurate. To handle this risk, we conduct additional process development to gain a level of confidence for a reliable product.

- A respondent from Norton:

We manufacture a family of materials made from silicon nitride. These ceramic materials are used in applications that include ball bearings and engine components. The ceramic balls are used for bearings in dental drills, machine tools and rocket exhaust systems. Our balls when used as bearings have long operational lifetimes under stressful conditions. One of our recently developed ceramic ball materials was recognized by the American Ceramic Society with its corporate Technical Achievement Award.

We use the PDFC volumes for research and development of new material formulations to improve properties such as toughness, high temperature strength and creep resistance. We investigate the interactions between different oxides, as an example. Our research results in a continuous improvement of materials used in our products. As product and market opportunities develop, we can select from our portfolio of materials to meet the needs of our customers.

The use of the PDFC is almost continuous through the various stages of the product life cycle, and they are used most often in the early stages. About 90 percent of our new product developments benefit from the PDFC data. In lieu of the PDFC volumes, we would search the technical literature for non-evaluated equilibria data. We could not afford the other options, such as internal experimentation, since we would need an army of people. The evaluated phase diagrams are very useful, and we hope that NIST continues with its Phase Diagram program.

- A respondent from Vesuvius:

The first product example involves ceramic refractories used in ferrous and nonferrous molten-metal applications. The key to developing this product involves understanding the temperature at which liquid forms in silicon nitride-based materials. The PDFC volumes have been used in all aspects of the product life cycle (research, new product selection, product design/development, and failure analysis). Research started on this product in 1992, the first prototypes were developed in 1994, and the product was introduced to market in 1996. Without the PDFC, this product likely would have arrived on the market three years later. Moreover, about 50 percent of our refractory ceramics have benefited similarly from the PDFC Volumes.

The second product example involves using silicon nitride in the chlorination process for purifying and refining gold. Chlorine reacts with the several contaminants of gold (copper, lead, nickel, zinc, cadmium, silver, etc.) to form a variety of chlorides (e.g., copper chloride). Some chlorides become volatile at gold melting temperature and others become liquid, resulting in slag formation. Understanding the interactions between silicon nitride and

the chloride slag is the key to developing this process. Much of this data is compiled in the phase diagrams. We first spent several days looking at the older diagrams (first four PDFC volumes) that show combinations of various compounds with only one or two anions. But, we ultimately found more data in the recent PDFC volumes that show phase diagrams with a wide variety of combinations of oxides, chlorides, nitrides, metals, salts, and gases.

We need the recent PDFC volumes for failure analyses in our current projects to improve the products we are selling. Our most recent work begins to address new formulations that could benefit from even more PDFC volumes as we're moving into difficult, uncharted territory with certain chlorides, oxides, nitrides, sulfides, carbides, and different compounds of these anion groups. This work is not thermodynamically pure, but the phase diagrams would be useful on an experimental basis.

The PDFC volumes are our most fundamental reference and all of our engineers use them. Without the phase diagrams we would be shooting in the dark in most of our problem-solving efforts. One of the benefits of the phase diagrams is that we can eliminate unnecessary experimentation. In lieu of the evaluated diagrams, we would need an extra person for the duration of every major project to account for such additional experimentation. Across all of our corporate activities, this would translate to five or six extra engineers every year.

Periodically, we get involved with non-evaluated phase diagrams, particularly in dealing with patent claims. In some cases, an experienced engineer can quickly resolve the uncertainties of such diagrams. In other cases, we have expended considerable time and money on consultants and in-house research in the assessment of these non-evaluated diagrams to resolve certain business issues.

## **4.2 ESTIMATES OF COMPANY BENEFITS**

An estimate was made of the additional annual cost each company would incur in steady state for adjusting to the hypothetical counter-factual environment in which no evaluated phase diagram information existed. These estimates were based on lengthy discussions with each company respondent about the cost of pursuing the described R&D projects in the absence of the PDFC volumes and the frequency of such occurrences. In most cases these estimates were formulated during the interview so that the accuracy of the estimate could be verified. The following situation typifies the nature of these conversations:

Company XYZ uses the PDFC volumes in about 40 percent of its research activity and product design/development activity. In the absence of such evaluated data (e.g., in the absence of any future research to evaluate phase diagrams at NIST), one to two additional person-years of effort would be needed each year to maintain the same quality of product

and the same production schedule. Valuing a ceramics researcher at the fully-burdened rate of \$200,000 per year, this company would incur a permanent increase in cost of \$300,000 ( $\$200,000 \times 1.5$  person-years) to maintain the status quo.

Many respondents of small as well as large companies stated that, in all likelihood, their firm could not carry such additional costs. Therefore, quality, reliability and/or new product introductions would fall.

The estimates to this hypothetical counter-factual question ranged from a low of \$3,000 per year to a high of \$1.7 million per year in additional labor and equipment costs. For 22 of 28 companies that were willing to engage in this estimating exercise, the sum of the steady-state additional annual costs is \$6.467 million. These 22 firms account for about 50 percent of the sales in the structural ceramics industry. Accordingly, the estimated sum of additional annual costs for the 22 companies has been extrapolated to the structural ceramics industry as a whole. Thus, \$12.934 million is a point estimate of benefits for this industry. This estimate is fundamental to the formulation of total industry benefits (cost savings) associated with NIST's research in evaluating ceramic phase diagrams.

Based on information from the interview process, the 22 firms in the sample size apply the PDFC volumes in a manner representative of the remaining firms that constitute the structural ceramics industry. Regardless of the size of the firm, phase diagrams are used in approximately the same product stages and with the same intensity. Also, regardless of firm size, typically only one or two engineers/scientists in each firm make use of the phase diagrams. Based on this information, albeit subjective, the benefits of the sample group have been extrapolated to the entire industry based on a sales-related coverage ratio of 50 percent. While an argument can be made that a benefits extrapolation based on numbers of firms rather than on sales and market share is more reasonable, the latter method of extrapolation provides conservatism to the estimate of industry benefits. Further, many of the firms in the sample size also market products in the other three market segments (electronics, environmental, and coatings) of the advanced ceramics market. The benefit data obtained in the survey appears to extend over the products for these markets.

## 5.

## ECONOMIC ANALYSIS

### 5.1 COST AND NET BENEFIT DATA

Table 4 shows the data used for the economic impact analyses. Total expenditure data from NIST for fiscal years 1985 through 1996 have been reproduced from Table 1. According to the management of the Phase Equilibria Program, the portion of research costs related specifically to advanced ceramics are inseparable from the total Program expenditures. Thus, these cost data include the costs of outputs beyond the scope of the study. These inflated cost data provide a downward, conservative bias for the calculated metrics.

**Table 4 NIST Costs and Net Industry Benefits (current \$000)**

<b>Fiscal Year</b>	<b>NIST Costs</b>	<b>Industry Benefits</b>
1985	420	-----
1986	420	-----
1987	382	-----
1988	294	-----
1989	255	-----
1990	265	-----
1991	87	-----
1992	94	-----
1993	103	-----
1994	105	-----
1995	97	-----
1996	136	-----
1997	0	12,934
1998	0	13,241
1999	0	13,556
2000	0	13,878
2001	0	14,207

Also shown in Table 4 are estimates of annual industry benefits associated with avoiding additional resources to maintain the same product quality and production schedule in the absence of NIST's evaluated data in the PDFC volumes. The data are based on the 1997 point estimate of net industry benefits totaling \$12.9 million (see Section 4.2) which has been extrapolated through 2001. This five-year time frame for forecasting cost savings is not arbitrary. A number of the respondents who had institutional knowledge



about their company stated during the telephone interviews that their company's product mix had tended to change over the course of about five to ten years. Thus, a five-year projection to define steady state appears reasonable.<sup>10</sup> These yearly benefits have been increased by an annual inflation factor of 2.375 percent.<sup>11</sup>

For evaluation purposes only, zero economic benefits to industry have been assumed over the years 1985 to 1996. Obviously, this is an unrealistic assumption based not only on common sense but also on the survey responses. To illustrate, one survey respondent noted the recent use of the PDFC volumes:

Our company makes ceramic materials that are manufactured into wear-resistant parts by our customers. The phase diagrams contain important information correlating melting points with the wear resistance properties. Our research began in 1991, the prototype appeared in 1992, and the product was introduced to the market in 1993.

However, no quantifiable information emerged from the survey interviews to facilitate an estimate of benefits prior to 1997. The omission of these pre-1997 benefits provides downward bias for the economic analysis.

Certain costs associated with the diffusion of NIST's research outputs are not included in this economic analysis. An implicit assumption is made that the publishing costs incurred by ACerS, as noted in Section 1.3, are offset by the revenues that ACerS receives from the sale of the PDFC volumes to the population of ceramics researchers. As stated previously, the focus of the economic analysis is to quantify the economic benefits attributable to NIST's evaluations net of ceramists' costs to purchase the related volumes.

## 5.2 MEASURES OF ECONOMIC IMPACT

The return that industry receives from investments made through the NIST Ceramic Phase Equilibria Program has been calculated using four widely-accepted measures of economic impact. These evaluation measures are the internal rate of return, the implied rate of return, net present value and the benefit-to-cost ratio.

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<sup>10</sup> In the extreme case of assuming this benefit stream would last continuously, the capitalized estimate of benefits in steady-state is \$86.2 million. This estimate is based on an opportunity cost of 15 percent — a hurdle rate characteristic of the private sector.

<sup>11</sup> An approximation of inflation is based on the implicit price deflator of the chain-type weighted Gross Domestic Product (GDP) Price Index. Based on data from the Bureau of Labor Statistics, the implicit price deflator is 2.375 percent.

### 5.2.1 Internal Rate of Return

By definition, the internal rate of return (IRR) is the rate of discount that causes a series of costs and receipts to approach proportionate equivalence. Applying this concept to the evaluation of research projects, the IRR is the discount rate that reduces the net present value (NPV) for a stream of expenditures and net benefits to zero. Mathematically, the IRR is the discount rate  $r^*$  that satisfies the equation:

$$NPV (r^*) = \frac{(B_0 - C_0)}{(1 + r^*)^0} + \dots + \frac{(B_t - C_t)}{(1 + r^*)^n} = 0$$

where  $(B_t - C_t)$  represents net benefits in year  $t$ , and  $n$  is the number of years for the research project. Reducing NPV equal to zero is comparable to a benefit-cost ratio of one (the break-even point), which allows comparisons of IRRs among projects of different sizes. The IRR equation is then rewritten as:

$$NPV (r^*) = \sum_{t=0}^n \frac{B_t}{(1 + r^*)^t} - \sum_{t=0}^n \frac{C_t}{(1 + r^*)^t} = 0$$

and,

$$\sum_{t=0}^n \frac{B_t}{(1 + r^*)^t} = \sum_{t=0}^n \frac{C_t}{(1 + r^*)^t}$$

Based on the stream of cost and net benefit data for fiscal years 1985 through 2001 in Table 4, the calculated value of  $r^*$  that equates NPV to zero is 0.335 (rounded).<sup>12</sup> In other words, 0.335 is the lower-bound value of the discount rate that equates the present value of benefits to the present value of costs. This implies a lower-bound internal rate of return of 33.5 percent for NIST's investments in evaluations of ceramic phase diagrams.

### 5.2.2 Implied Rate of Return

Under an alternative set of assumptions, an implied rate of return is calculated from the data in Table 4.<sup>13</sup> For example, if all of NIST's costs are referenced to 1985 using a nominal discount rate of

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<sup>12</sup> The data in the first year of the benefit-cost stream are referenced to time  $t=0$  in the IRR equation as well as for the other economic measures.

<sup>13</sup> The implied rate of return is similar to the overall rate of return suggested by Rosalie R. Ruegg and Harold Marshall, *Building Economics: Theory and Practice*, (Van Nostrand Reinhold: New York, 1990). An

9.375 percent as recommended by the Office of Management and Budget, then the present (1985) value of NIST's costs is \$1.94 million.<sup>14</sup> When all industry benefits are referenced forward to the year 2001 using the same 9.375 percent discount rate, the terminal (2001) values of industry benefits are \$81.4 million (lower-bound) and \$195.9 million (upper bound). Using the implied rate of return, the NIST TCP is viewed as a single calibration project where an initial net investment of \$1.94 million generated, after 16 years, a consumer surplus equaling \$87.4 million (lower bound) and \$195.9 million (upper bound). Thus, the annual compounded rate of return corresponding to such an initial investment in 1985 that culminates in 2001 is based on the value of  $i^*$  that satisfies the following lower-bound relationship:

$$\$1.94\text{M} (1 + i^*)^{16} = \$81.4\text{M}$$

In this case, the calculated value of  $i^*$  equals 0.263 which means that the lower-bound implied rate of return for the NIST research activity on ceramic phase diagrams is 26.3 percent

The IRR is often confused with the implied rate of return. Both measures are used in financial analyses but the type of cash flow pattern associated with the implied rate of return occurs neither in an R&D project, in general, nor in the case of NIST research and activities related to phase diagrams, in particular. Therefore, the implied rate of return is not directly comparable to the IRR discussed in the economics literature.

### 5.2.3 Benefit-to-Cost Ratio

A benefit-to-cost ratio (BCR) relates the present value of NIST research costs to resulting industry benefits. The calculation of a BCR is based on the following formula:

$$NPV (r^*) = \sum_{t=0}^n \frac{B_t}{(1 + r^*)^t} - \sum_{t=0}^n \frac{C_t}{(1 + r^*)^t} = 0$$

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example of the implied rate of return, also known as the compound rate of return, is the annual yield earned on a \$100 bank deposit. Interest is earned each year on the original \$100 plus compounded interest.

<sup>14</sup> "Guidelines and Discount Rates for Benefit-Cost Analysis of Federal Programs," Office of Management and Budget (OMB), Circular No. A-94, 29 October 1992. OMB recommends both a seven percent real rate of discount for federal project evaluations and an approximation of inflation based on the implicit price deflator of the chain-type weighted Gross Domestic Product (GDP) Price Index. Based on data from the Bureau of Labor Statistics, the implicit price deflator is 2.375 percent which is used to convert the real discount rate of seven percent to a nominal rate of 9.375 percent.

For this case study, costs and net benefits are deflated to the base period (1985) using a 9.375 percent rate as in the implied rate of return calculation. Using 1985 present values of costs (\$1.94 million) and the present value of lower-bound benefits (\$19.4 million), the calculated BCR is 10.0 to 1.

## 6.

## CONCLUSIONS

This case study provides evidence on the economic importance to the domestic ceramics industry of NIST investments for evaluating ceramic phase equilibria diagrams. Industrial representatives provided an array of anecdotal insights on the practical use of phase diagrams throughout the product life cycle.

The hypothetical, counterfactual experiment shows that, in lieu of NIST's investments, ceramic manufacturers collectively would be less efficient in attaining comparable technical data. Ceramists would incur greater costs for internal research and experimentation. These additional costs would likely be passed on to downstream manufacturers and ultimately, to the consumers of ceramics-based products. Also, delays of six months or more would occur in introducing innovative ceramic materials to market. Such economic inefficiencies would certainly have an adverse effect on the international competitiveness of U.S. ceramic component suppliers.

Several factors have been incorporated in this study to characterize the lower bound estimates of the IRR, BCR and implied rate of return calculated in Section 5.2 as conservative estimates of NIST's economic impact on industry. These factors are:

- The scope of the study did not account for benefits realized by other firms in the industry structure (horizontally and vertically) external to the advanced structural ceramics industry
- Extrapolation of benefits from the sampled firms to the larger set of firms in the structural ceramics industry was based on sales and market share data rather than a multiplication of the average benefits per firm from the sample times the number of firms in the industry
- Due to imprecise accounting records, NIST's cost data includes expenditures for outputs beyond the scope of this case study, thereby biasing the results downward
- The 1997 starting point adds to a conservative benefit estimate since industry attains benefits from NIST's investments in prior years (1985-1996) of the economic framework for this study

Economists and policy makers use IRR measures to estimate the social rate of return (SRR) for on-going or completed research projects in the public sector. If the 33.5 percent IRR in this case study is above NIST's hurdle rate (minimum acceptable rate of return), then the investments in NIST's research and related activities are worthwhile from a social perspective.

# **APPENDIX A**

## TECHNICAL OVERVIEW OF CERAMIC PHASE EQUILIBRIA DIAGRAMS

### DESCRIPTION<sup>16</sup>

An understanding of phase equilibria relations (the positions in phase diagrams where various points, lines, or surfaces of phase reactions occur under equilibrium conditions) is basic in the development and utilization of ceramic materials used in advanced applications.<sup>17,18</sup> Phase equilibria address the flexibility and constraints dictated by forces of nature on the evolution of phase assemblages in ceramics. Phase boundaries also assist in the evaluation of the service stability of a ceramic material, both in the long and short time frames. Thus, knowledge of the stability of a ceramic component in high-temperature or high-pressure environments can often be obtained from an appropriate stable or metastable phase diagram.

Phase diagrams yield important information on key processing parameters of ceramics. The chemical and physical properties of ceramic products are related to the number, composition, and distribution of the phases present. Temperature, pressure, and material concentration are the principal variables that determine the kinds and amounts of the phases present under equilibrium conditions. To ceramists, who must understand the effects of these variables on both the processing and the properties of finished ceramic products, the necessary fundamental information of phase equilibrium relations is often provided from phase diagrams.

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<sup>16</sup> This section is based on the following: Clifton G. Bergerson and Subhash H. Risbud, *Introduction to Phase Equilibria in Ceramics* (The American Ceramic Society), 1984, p.1; Floyd A. Hummel, *Introduction to Phase Equilibria in Ceramic Systems* (Marcell Dekker), 1984; and The McGraw-Hill Encyclopedia of Science and Technology, 7th edition, 1992.

<sup>17</sup> Phase equilibrium is a general field of physical chemistry concerning the various situations that occur with the coexistence of two or more phases in thermodynamic equilibrium, the nature of the transitions between these phases, and the effects of temperature and pressure on these equilibria. A phase is any physically-homogeneous portion (state of aggregation) of a system which is bounded by a surface that is separable mechanically from any other portions (phases) of the system. The term “system” refers to an isolated part of the material universe for considering changes that occur under varying conditions. From a thermodynamic standpoint, a system that has a minimum of free energy available for doing work is at equilibrium.

<sup>18</sup> Ceramics are inorganic, nonmetallic materials that are produced typically by using clays and other minerals from the earth, forming these materials into a desired shape, and heat treating in order to obtain a rigid, finished product. They are typically crystalline in nature (the exception being glasses) and are compounds formed between metallic and nonmetallic elements such as oxides, nitrides and carbides. Also, they are typically insulated to the passage of electricity and heat, and are more resistant to high temperatures and harsh environments than metals and polymers. Regarding mechanical behavior, ceramics are very strong in compression but weak in tension — they are very hard but tend to be brittle.



The phase diagrams provide reference data that represent the phase relations under a certain, limited set of conditions (for example, constant pressure). A ceramist conducting new materials research will invariably conduct experiments under different conditions than those that underlie the phase diagram. The reference data in the phase diagram provides the user with a logical place to begin experimentation for new research and to bypass certain paths that would lead to dead ends. This practical use of the diagrams helps explain why the PDFC volumes just show the actual diagram and a brief textual description without any accompanying tabular data.

Figure A-1 shows a simple binary diagram that depicts the phase relations between magnesia and lime, or calcia. A binary phase diagram plots temperature on the vertical axis and composition, or the percentage of the two material components, on the horizontal axis. The diagram is basically a simple graphic representation of a large amount of chemical thermodynamic data.<sup>19</sup>

One of the primary inferences from the phase diagram is the phases present at a given temperature and composition. For example, pure magnesia melts in excess of 2,800 degrees centigrade (°C) and lime melts in excess of 2,600 °C. However, if magnesia and lime are in contact with each other at temperatures as low as 2,400 °C, then the phase diagram shows that the two solids are unstable and they will react to form a liquid phase. This kind of information is extremely useful in understanding the compatibility of materials, particularly at high temperatures, and is one of the main reasons why phase equilibria are so important to ceramics since they are used primarily at elevated temperatures.

Most ceramic systems tend to be considerably more complex than the previous system described. Figure A-2 shows a projection of the liquid surfaces of the calcium oxide, silica, aluminum oxide (CaO-SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>) system. This diagram shows the complexity that exists in real ceramic systems. For example, several binary compounds exist between each of the end-points along the edges of the ternary triangle, and several compounds are within the interior of the ternary diagram. This particular diagram, known as “the million dollar diagram” in the ceramic industry, is important because of its preeminence to the cement and refractory industries. The highlighted portion of the same CaO-SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> diagram shown in Figure A-3 represents a wide range of refractory compositions used in all metals industries, glass production, and nearly every thermal insulation application. The ability of the refractories used in these furnaces to withstand high temperatures depends strongly on accessible and accurate phase diagrams.

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<sup>19</sup> Dick Spriggs, “ACerS Phase Diagram Program,” unpublished manuscript, July 1988.

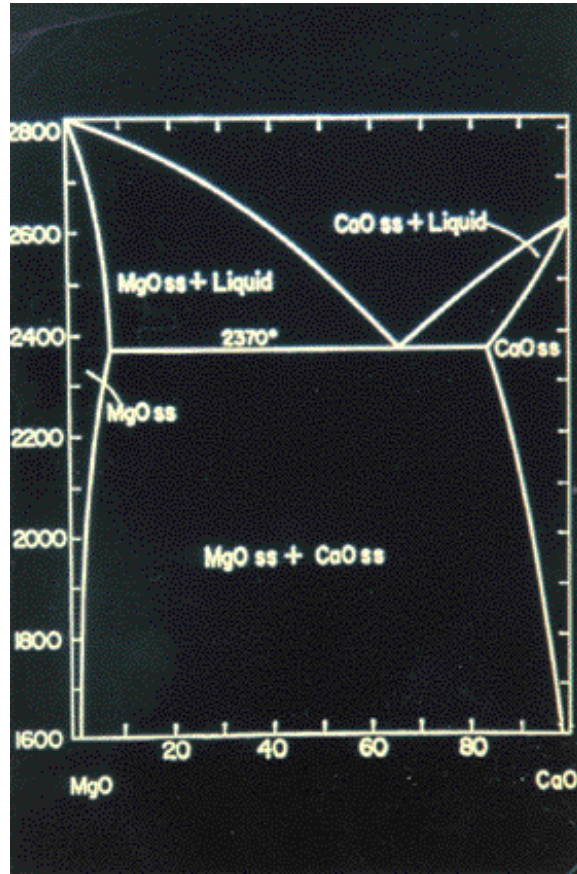


Figure A-1 MgO – CaO System

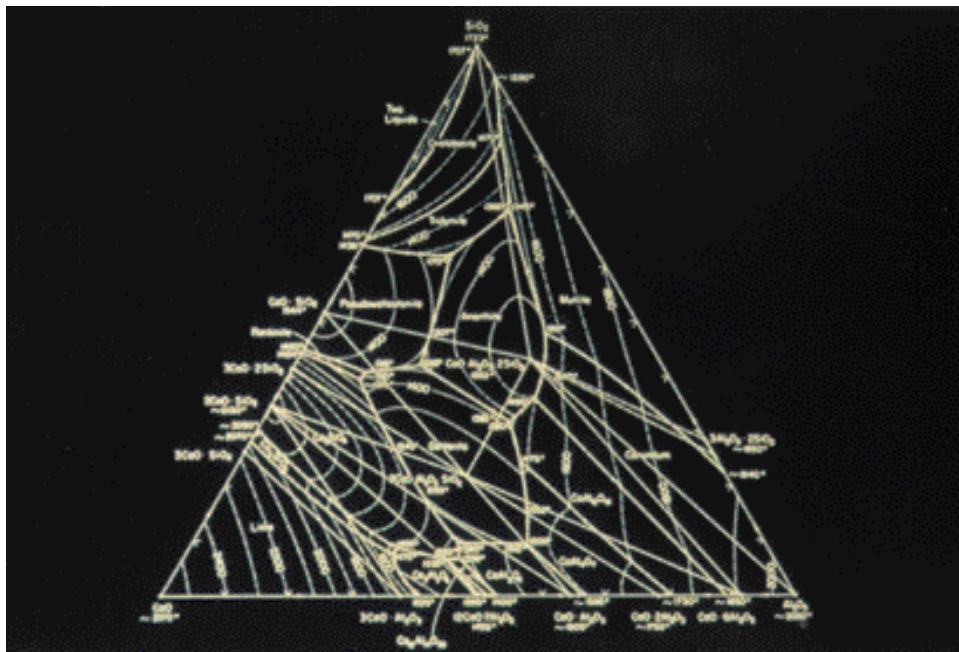
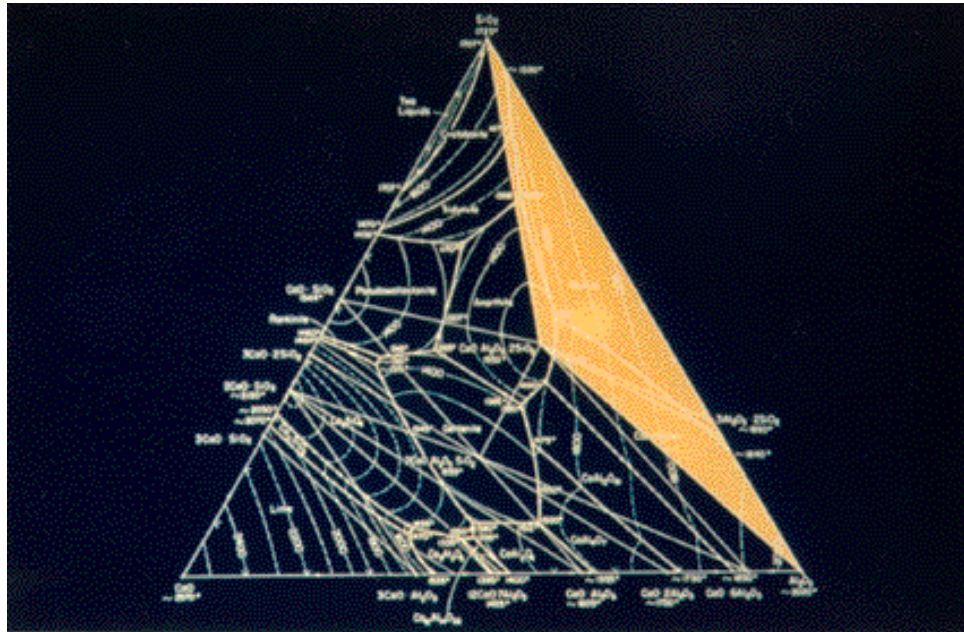


Figure A-2 CaO – SiO<sub>2</sub> – Al<sub>2</sub>O<sub>3</sub> System



**Figure A-3 CaO – SiO<sub>2</sub> – Al<sub>2</sub>O<sub>3</sub> System**

## METHODS OF DETERMINATION <sup>20</sup>

Ceramic phase equilibrium diagrams are the product of experimental studies of phase relations in a selected pressure-temperature-composition region of a system. These studies are categorized by two general methods: (1) static, and (2) dynamic. Static methods, such as quenching, use a specimen held under constant conditions at high temperature until equilibrium is reached, when the number and composition of the phases present are analyzed by microscopy at room temperature. Dynamic methods tests, such as thermal analysis or high temperature x-ray diffraction, characterize the appearance or disappearance of phases in the specimen directly during the heat treatment. Yet, typically, no one technique of studying phase equilibria in a system is completely satisfactory; rather, the final phase diagram is often based on information derived from several methods.

The diagrams represent the results of difficult and extensive experimental observations and analyses. For example, a binary system takes about one man-year of experimental effort, assuming the timely availability of the required equipment and the investigator is reasonably experienced. A ternary

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<sup>20</sup> This section is derived mainly from the unpublished manuscript by Robert S. Roth, "Experimental Determination of Phase Equilibria Diagrams in Ceramic Systems," 1988.

diagram can involve several thousand observations over a two-three year period after knowledge of binaries is reasonably complete. More complex systems require more extensive time and effort.

The “quality” of a phase diagram is affected by several factors. One factor that skews the results of the diagram is the level of experience and education of the experimentalist. Diagrams are also strongly dependent on both the type of experimental data accumulated and the sophistication of the instrumentation utilized. Another factor is that the original experimentalist may only be concerned with some limited region of composition, temperature, and pressure. When the experimental effort has been concentrated in that particular area, the other parts of the phase diagram are often determined with much less precision and detail.<sup>21</sup> For all these reasons, a phase equilibria diagram for a given system tends to change over time. Diagrams are subject to constant revision as additional measurements are made by subsequent researchers. As more and better data are accumulated by subsequent experimentalists, the diagram becomes more representative of the true equilibrium conditions.

A user of a phase diagram needs an explicit description of the experimental basis employed by the originator of the diagram. Such knowledge of the original methods used in determining the diagram and conducting measurements is especially important for users with critical and high-accuracy applications.

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<sup>21</sup> According to Roth, “Oftentimes, the exactness of the information presented in all parts of the diagram is not included in the summarization descriptions that accompany the diagram. As a result, a user can rely often on the general configuration of a given diagram, but the exact temperatures and compositions of individual lines or points on the diagram may not be totally reliable.”