Computerization and Networking of

Materials Databases

FIFTH VOLUME

Satoshi Nishijima and
Shuichi Iwata, editors

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Foreword

This publication, *Computerization and Networking of Materials Databases: Fifth Volume,* contains papers presented at the Fifth International Symposium on Computerization and Networking of Materials Property Data, held in Tsukuba, Japan on 6–8 Nov. 1995. The symposium was sponsored by ASTM Committee E49 on Computerization of Material and Chemical Property Data and the National Research Institute for Metals (NRIM), Japan.

The symposium chairmen were Dr. Satoshi Nishijima, NRIM, and Professor Shuichi Iwata, The University of Tokyo. They served as editors of this publication. S. Nishijima and S. Iwata acknowledge the significant contributions brought by Crystal H. Newton of Materials Science Corporation, who served as International Advisor for the Symposium. They are also grateful for the valuable assistance of Timothy M. King and Yoshio Monma of the National Research Institute for Metals.

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Overview

The present volume documents the proceedings of the Fifth International Symposium on the Computerization and Networking of Materials Property Data, held at the National Research Institute for Metals (NRIM) from 6 to 8 Nov. 1995, under the joint sponsorship of ASTM Committee E49 on Computerization of Material and Chemical Property Data and NRIM. In 1986, Committee E49 initiated its standardization activities to unify the efforts made by various individuals and to facilitate the building of materials databases as compatible media in engineering. At the same time, the Committee organized a series of International Symposia to explore the *state of the art* of relevant technologies every two years.

The first two symposia focused on the production of materials data and the next two on the utilization of data, as noted by the editors of the last volume in their overview. This fifth meeting provided an opportunity to review and rearrange these developing data systems. Speakers at this symposium emphasized the significance of their philosophy and methodology to utilize their materials information and data. They discussed various technologies for the scientific prediction of materials behavior through expert systems and/or virtual experiments assisted by knowledge systems; the application of modern communication systems such as the Internet have become popular and were introduced in many systems.

The papers in this volume were grouped to help provide an understanding of the different technological fields.

Materials Science and the Role of Virtual Experiments

Tomiura presented an overview paper, "Lessons from a Case Study of Property Databases in Materials Development." The author is a senior Japanese Industrial researcher who through a long career has seen the use of computers develop to support materials research and development in industry. The examples in the paper illustrate that the computer can support the application of materials science knowledge for effective engineering. However, some solutions are not fully successful because of limitations in data and software technology.

Nishikawa et al. presented a paper called "Integration of Virtual Experiment Technology for Materials Design," The application of computers to materials engineering has achieved progress mainly in a single technology. This paper discusses the foundations for an approach that attempts to establish integration of individual successes. The inevitable progress of hardware will provide the necessary speed, but the challenge for materials technologists is to ensure the accurate collaboration of software that provide functions such as databases, numerical analysis, and knowledge processing.

Inaba discusses issues of "Control of Metal/Oxide Interface Reactions by the Use of Chemical Potential Diagrams." The development of materials science provides an analytical understanding of complex but important phenomena. Such an understanding is ideal for implementation in computer systems. This paper describes the possibility of predicting the reactions of multicomponent chemical systems. The computer is the ideal tool to support such numerical simulation and to provide the transfer of research achievements to the industrial materials engineer.

Progress and Refinement of Data Models

Ashby discusses engineering judgment for use of materials in his paper "Materials Selection: Multiple Constraints and Compound Objectives." The author emphasizes that the optimization of materials selection in design is usually overconstrained and frequently directed to conflicting objectives. He introduces a concept of material indices that can express a target function for a given mechanical component. He says that once the indices are determined, the selection is easy by comparing the materials data in a space having primary materials indices coordinates.

Ono discusses "An Experiment on Internet Material Database Service with MOOD-SX." As a new paradigm for software, object orientation is gaining wide recognition for the potential to express information in a way that seems to be a more flexible view of the world. The author has worked for several years to create a database that can represent the rich detail of materials research results. The paper shows that access to this database is now feasible on the Internet and thus able to provide powerful support for the comprehensive sharing of materials science knowledge.

King et al. discuss problems of materials models in "Towards a Flexible and General Computer-Based Representation of Experimental Data." Traditionally, software limitations have controlled the development of materials property databases. However, modern computer technology offers a new generation of developers greater freedom to ask questions about the fundamental nature of the data. This paper reveals the inherent flexibility when the data model does not recognize any potential limitations in the database software. Such approaches offer the prospect that materials scientists can more accurately express their understanding of the world and allow the computer to provide support of the engineering process.

Hiraoka reported the initial outcome of a long task in "STEP—Present and the Future." The paper introduces the outline of a new international standard, ISO 10303, known as STEP, that offers a computerized method of representing and exchanging product data. STEP defines geometry, configuration, drawing, material, and other aspects for a product and indicates the possibility of using these data in different computer systems such as Computer Aided Design (CAD) and Computer Aided Manufacturing (CAM) in a consistent way. The paper discusses several issues of this new attempt, especially the needs when developing good and usable product models.

Expert Systems and Knowledge Organization

Kawazoe et al. report the status of their system in "Multimedia Database System KIND Featuring Amorphous Factual Database by Object-Oriented Method." The authors' group has been developing a materials information system including literature and factual data on phase diagrams for ternary amorphous alloys. The paper introduces the outline of the system, designed to predict new amorphous-forming compositions by use of the object-oriented concept. The system is open to the public through the computer network and therefore will be judged as to its performance by external users.

Roberge and Trethewey wrote "Object Orientation for Fusion of Corrosion Data." The understanding of corrosion includes qualitative elements that are beyond representation by pure analytical methods. When reports contain natural language discussions of corrosion phenomena, the retrieval and combination of data are difficult. This paper shows the benefits of appropriate extraction and representation of nonquantitative knowledge. The computer is able to identify possible patterns and interpretations of data from many unrelated sources.

Minoshima et al. introduce their expert system in "Development of an Expert System for Fractography of Environmentally Assisted Cracking," with many similarities to the previous paper. When components crack in nonbenign environments, the influential factors are numerous and interact in a complex way. Thus, the research scientist finds it difficult to express rules in a strict analytical fashion. This paper presents some of the modern software technologies that have capabilities to represent nonquantitative knowledge.

Sturrock and Bogaerts report the results of an extensive study in "Classification and Prediction of the Corrosion Behavior of Nickel-Containing Alloys from Field Test Data." The subject of this paper is related to decision-making strategy in engineering based on some sort of data but having large scatter. The data in this case are field corrosion test data that are often of a multi-dimensional nature. Among various statistical methods they investigated, the nearest neighbor method provides the best performance when used in combination with decision trees and the polynomial networks approach.

Munro reports his experiences in "Expert System Technology for Natural Gas Resource Development." The discussion focuses on the exploitation of unconventional gas reserves: the possibility of extending existing expert systems is assessed for such particular cases. It suggests that an expert system may be a more powerful tool if the surrounding technical premise can be appropriately extended according to the real situations.

New Aspect of Data Content, Data Evaluation

Halada et al. introduce a new concept in "Database for MLCA (Materials Environmental Life Cycle Analysis)." Recently, public opinion has brought pressure on engineers to consider more carefully the impact of industrial activity on the balance between humans and the natural environment. However, achieving an accurate assessment of this balance requires a very broad view of the engineering process. The application of information technology offers the prospect of broadening this view. This paper shows the variety of necessary materials data and the principles by which to evaluate the environmental impact of materials engineering.

Oland and Frohnsdorff discuss the complexity of materials models in "Guidelines for Identification of Concrete in a Materials Property Database." The paper introduces guidelines to describe concrete materials using a logical scheme for organizing and subdividing various information on the property and its constituents. The guidelines also provide for data reporting and therefore for the building of related databases.

Munro and Chen discuss data evaluation issues in "Data Evaluation Methodology for High-Temperature Superconductors." Many publications came out during the first years of research on high-temperature superconducting materials. Among them, there were many seemingly conflicting results, as is generally the case for an engineering field that is immature. This paper proposes a methodology to evaluate data in the literature using a structured procedure that can be helpful for other applications. The procedure applies to each set of data and leads to assigning the class of data as certified, validated, evaluated, and so on.

Yamamoto et al. illustrate the use of a database to manage long field tests in "A Corrosion Database System for Exposure Tests." The system controls various steps of field corrosion tests that are to be continued for many years in industry. The advantage of the system is to conduct long and complicated experiments without problems even when a change of operator takes place, and, of course, to analyze progressing results when needed. A system of this kind would provide even more of a benefit if a communication link is established between similar systems in different organizations.

Nakayama et al. introduce a group project on database development in "Strength Characteristic Analysis Using the Database for Mechanical Properties of P/M Alloys." The data are mainly on the strength of ferrous and aluminum alloys that are used for mechanical parts. The database contributes to the improvement and research of those materials properties.

Advancement of Computer Technologies

Sandström and Komenda emphasize the significance of microstructural information of materials in "Materials Database with Microstructural Information." Many properties such as mechanical strength have an essential correlation with microstructures. This paper introduces a representation of microstructures both in qualitative and quantitative form suitable for materials property databases. Automatic image analysis allows combining micrographic information with other metallurgical data in a comprehensive way.

Fujita et al. reported a similar work, "A Distributed Database System for Mutual Usage of Materials Information (Data-Free-Way)." This paper introduces the effort to develop a computerized system representing microstructures of engineering metallic materials in quantitative and qualitative ways. An automatic image analysis system classifies microstructures by characteristic parameters such as; size and shape of grains, particles, inclusions, voids, bands, all incorporated in a database with micrographic images of the material. The whole system is ongoing and success will rely on how properties of engineering significance can be correlated to the microstructures.

Yokoyama et al. report a database working across the Internet in "Development of Comprehensive Material Performance Database for Nuclear Applications." The system supports data entry as well as query and analysis of data. It shows that the technique is now popularized and no longer the sole domain of specialist companies.

Fujiwara et al. briefly sketch a proposal in "Materials Information Systems for Open World Problem Solving." It is true that modern materials R&D has the tendency to require information that is more and more specialized and complex. No conventional data and/or knowledge system can satisfy users in an ideal manner. The author indicates that the self-organization of information would be a solution for this purpose. The goal of the problem, however, seems far off.

To summarize, one can say that the methodology to utilize materials data and information systems has progressed significantly in recent years. Challenges have resulted in *autonomous systems* by introducing, for example, human interventions in the multi-directional information exchange between users and producers. This trend will no doubt continue, helped by a recent drastic increase in those reaching these systems through the Internet. It is thus persuasive that this assures the advancement of related science and technology in a visible way.

Satoshi Nishijima

Center for Advanced Physical Fields, National Research Institute for Metals, Tsukuba; symposium chairman and editor

Shuichi Iwata

Research into Artifacts, Center for Engineering, University of Tokyo, Tokyo; symposium chairman and editor

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