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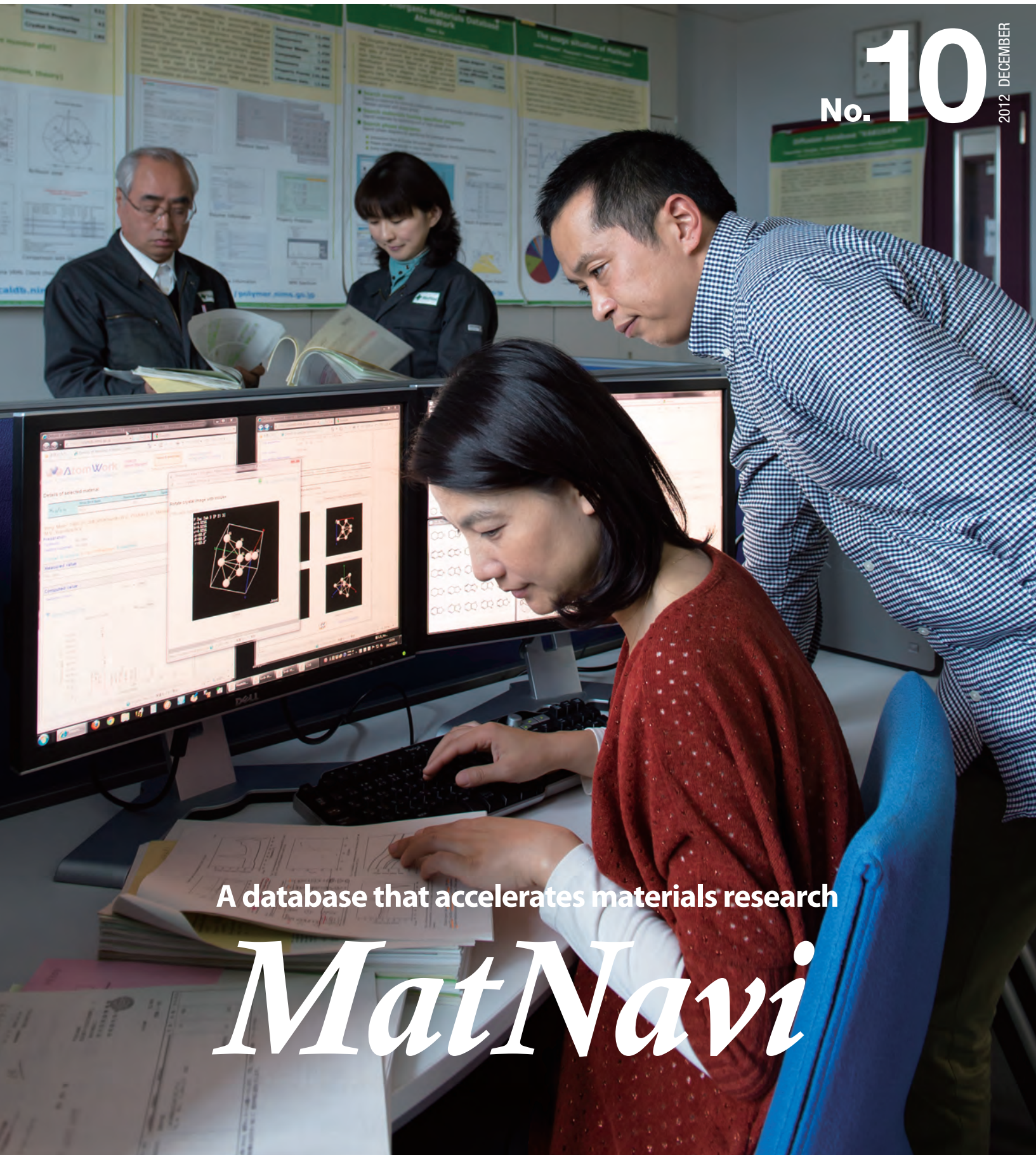

A database that accelerates materials research

MatNavi

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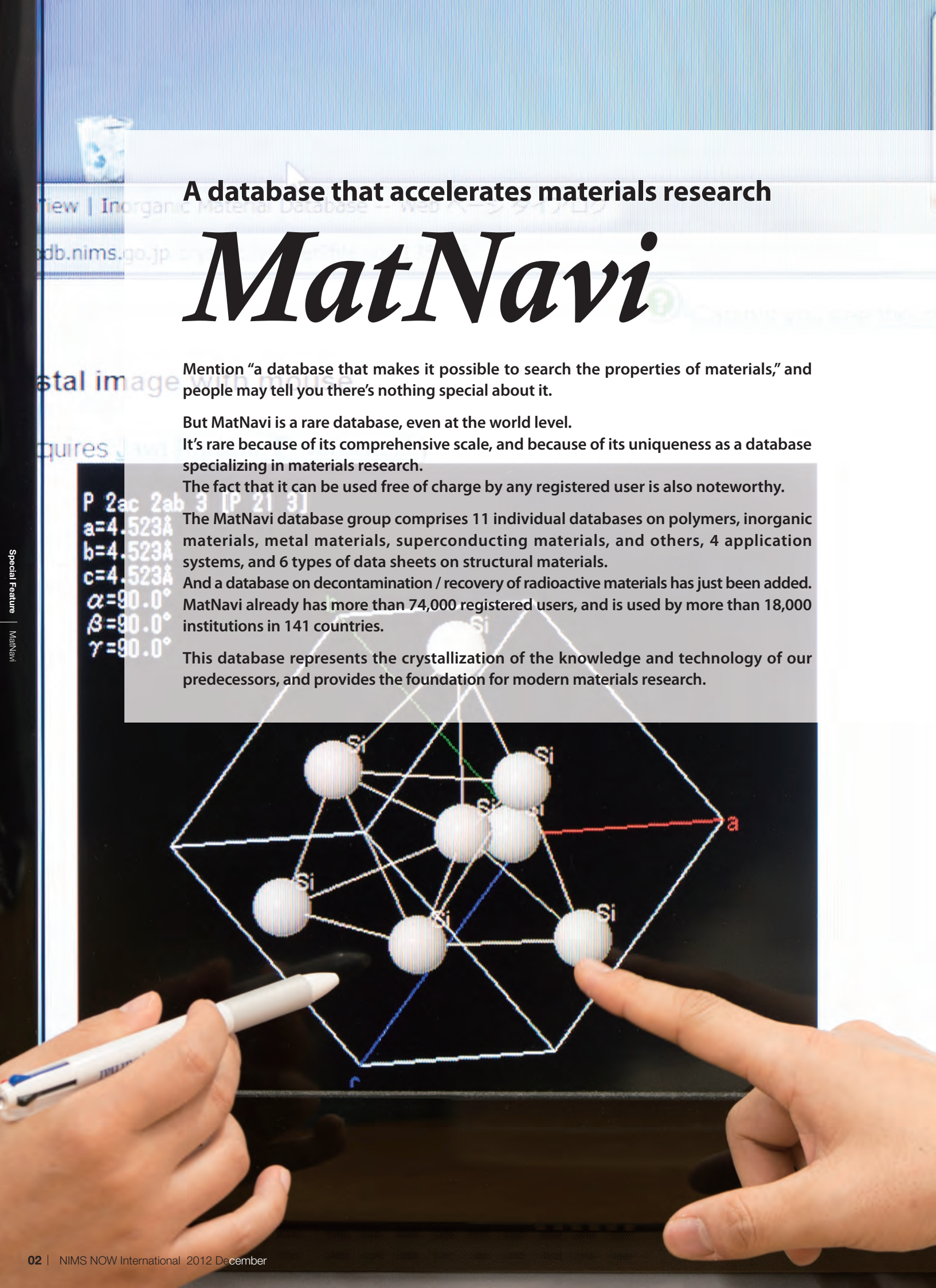
Mention "a database that makes it possible to search the properties of materials," and people may tell you there's nothing special about it.

But MatNavi is a rare database, even at the world level.
It's rare because of its comprehensive scale, and because of its uniqueness as a database specializing in materials research.
The fact that it can be used free of charge by any registered user is also noteworthy.

The MatNavi database group comprises 11 individual databases on polymers, inorganic materials, metal materials, superconducting materials, and others, 4 application systems, and 6 types of data sheets on structural materials.
And a database on decontamination / recovery of radioactive materials has just been added.
MatNavi already has more than 74,000 registered users, and is used by more than 18,000 institutions in 141 countries.

This database represents the crystallization of the knowledge and technology of our predecessors, and provides the foundation for modern materials research.



Special Message

MatNavi and combinatorial investigation of new functional materials

University of Maryland
Ichiro Takeuchi

If you look at the recent U.S. materials research scenes, there are many focused efforts on improving and discovering new materials targeting energy applications in sustainability related topics. There are also many discussions about designing materials and predicting new compounds based on computational materials techniques. The funding trend also reflects these focuses in the field.

My research group carries out combinatorial investigation of a variety of functional materials. We use thin film libraries to explore new phases of inorganic functional materials in specific topics funded by the U.S. Department of Energy and the Department of Defense. For example, we currently have projects looking for new rare-earth free permanent magnets. The goal is to find new magnets which can be used in motors of future generation electric and hybrid vehicles as well as direct drive wind-turbines.

Having a comprehensive database on previously explored materials is crucial for such exploratory investigation because one needs to be able to decide which new phase spaces to investigate. In most fields, such databases are not available. MatNavi's AtomWork is very unique in that it is based on a large collection of previously published references, and it can list relevant physical properties in easy-to-see tabulated formats. It is very rare to find such a resource available publicly.

For instance, when we started the projects on rare-earth free magnets, it was clear that there was a large body of references on compounds which previous researchers had worked on. Some materials are pretty common and famous compounds, but others are not. No one person can know of all possible materials which have been studied to date. It is extremely useful to see the extensive list in MatNavi. These days, whenever we think of a possible new material to try, we first check with AtomWork.

We are also using the SuperCon in MatNavi as a guide for our combinatorial search of new superconductors. Again, it provides a very powerful reference list of all superconductors ever studied. The database is so comprehensive that it lists up to 29,000 entries. Given that detailed properties from individual reference need to be entered, this represents an enormous amount of hard work by the MatNavi team. Another important aspect of SuperCon is that one can make a downloadable table of list of properties. Such a table can then be potentially used to carry out data-mining to look for hidden correlations between properties.

Because it is extremely time-consuming to construct such databases "manually," there have been discussions about incorporating machine-reading techniques to develop methods to automatically "read and extract" important physical property information from published papers. Although such an effort is in its infancy in materials science, I believe these techniques will be useful for constructing databases in the future.

If you survey the field of computational materials science, there are many groups using databases such as ICSD (Inorganic Crystal Structure Database) as a data-mining tool to carry out computations (of structural information) and to predict new stable compounds. Data available in MatNavi should be useful for such purposes also.

My group is still learning how to take full advantage of the enormous amount of information available in MatNavi. We are very grateful that it is open to public. Just as biological genomes are playing crucial and profound roles in medicine and biochemistry, I strongly believe that databases such as MatNavi will be the foundation of important materials research in the future.

Ichiro Takeuchi is Professor of Materials Science and Engineering and Affiliate Professor of Physics at the University of Maryland. Takeuchi obtained his PhD in Physics at the University of Maryland (1996). He was a Postdoctoral Fellow at Lawrence Berkeley National Laboratory (1996-1999). Takeuchi has previously served as Visiting Professors at the University of Tokyo, Tokyo Institute of Technology, Tokyo University of Science, and the Ruhr University, Bochum in Germany.

The NIMS Materials Database – MatNavi "The Value of a Database is in its Use!"

Station Director,
Materials Information Station,
Research Network and Facility Services Division
Toshio Ogata

Introduction

The NIMS materials database MatNavi is an online materials database of world's largest class. The MatNavi system comprises a total of 11 individual databases, such as the polymers database PoLyInfo, inorganic materials database AtomWork, and metal materials database Kinzoku, etc. It also has 4 applications, beginning with the composite materials thermal property prediction system CompoTherm, and online editions of NIMS Structural Materials Data Sheets, among information. It can be accessed by registered users free of charge at http://mits.nim.go.jp/index_en.html.

In recent decades, both the types and numbers of materials have increased by an order of magnitude, and as a result, today, materials databases are indispensable not only for appropriate selection of existing materials, but for development of new materials. Databases are also expected to respond to future increases in the number of substances and materials. Moreover, in addition to maintaining the hardware of those databases, it is also essential to update data continuously.

History of MatNavi

When the National Institute for Materials Science (NIMS) was launched in 2001, the functional materials database developed by the Japan Science and Technology Agency (JST) was also transferred to NIMS. Together with that database, NIMS also began integrated management of the databases inherited from one of its predecessor organizations, the National Research Institute for Metals (NRIM). Two years later, in April 2003, those databases were opened to public access via the internet under the name MatNavi. NIMS continued to improve the MatNavi database system, for example by integrating the server operating system and user authentication systems, while also working to reduce system maintenance costs. Subsequently, the server hardware and system were integrated to a certain extent, and the "New MatNavi" was opened to users in July 2010.

Concept of MatNavi

The individual databases of MatNavi can be accessed by registered users free of charge. Figure 1 shows the top page of MatNavi. MatNavi comprises the various types of databases operated and managed by the NIMS Materials Information Station and a horizontal search system for those databases, applications, materials information published by research groups at NIMS, links to the websites of institutes in Japan and other countries which provide materials databases, and other features. Figure 2 shows a list of the databases currently available at MatNavi. The polymers database PoLyInfo, inorganic materials database AtomWork, and metal materials database Kinzoku are introduced in the following articles, and information on other databases and details can be found in the feature article [1] shown below in the Reference.

To register as a MatNavi user, simply click New User Registration in the User Screen at the upper right of the main screen to open the Registration screen and enter the requested items. Your registered password will be sent back to you automatically at your email address. After once receiving user authentication, it is possible to access all the databases included in the MatNavi system.

In addition, the necessary data in all MatNavi databases can be located quickly by using the horizontal search system MatNavi Search.

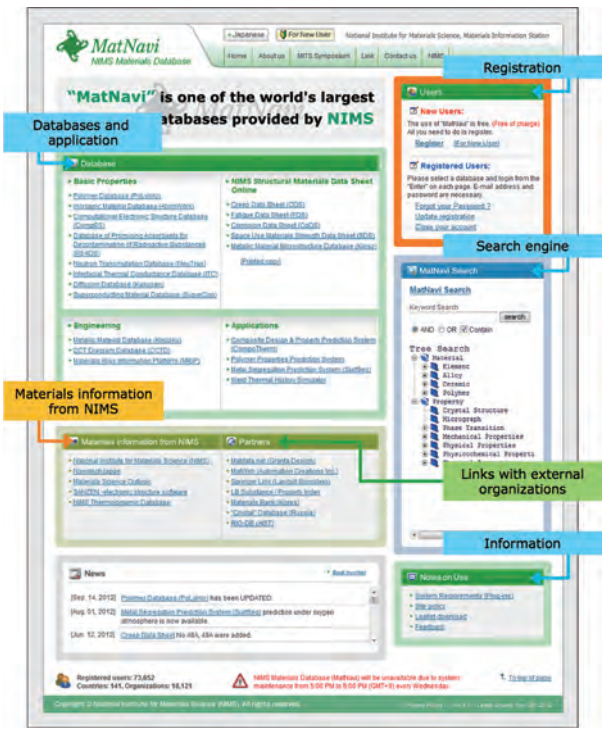


Fig. 1 Top page of MatNavi.

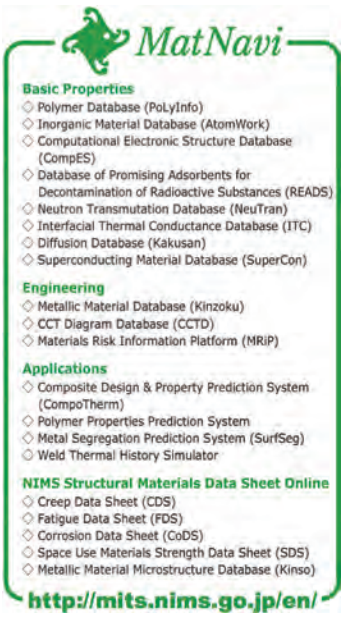


Fig. 2 Databases available at MatNavi.

Trends in registered users and access of MatNavi

Figure 3 shows the transition in the number of registered users. Each month, more than 2000 new users are authenticated and begin to use the MatNavi database. As of October 31, 2012, MatNavi had 73,652 registered users at 18,121 organizations in 141 countries. Of these, 53,487 were Japanese users, and 20,165 were users in other countries. This is more than a twelve-fold increase from the number when MatNavi opened in 2003.

Figure 4 shows the transition in the number of times the database was accessed for the MatNavi system as a whole. The average access rate since the new system opened in July 2010 is 1.2 million times per month, which is double the previous rate, and in October of 2012, this number exceeded 1.7 million. The most frequently accessed databases are the inorganic materials database, polymers database, and metal materials database.

Activities and evaluation of MatNavi

With the motto "The value of a database is in its use," we are constantly striving to provide the most complete data possible, while also incorporating new advances in IT and server hardware.

Approximately 40% of our users, both in Japan and other countries, found MatNavi through general search engines like Google, Yahoo, goo, etc. MatNavi is the top hit in searches for "Materials database" in Japanese, and is always shown on the top page in searches for "Materials database" in English. Thus, in both name and reality, MatNavi ranks in the world's top class of materials databases.

Among activities, in December 2011, NIMS held a MITS Database Symposium in Akihabara, Tokyo, which attracted more than 150 participants. In April 2012, the 3rd Asia Materials Data Symposium, centering on Japan, China, and Korea, was held in Naha on the island of Okinawa, and this event also attracted more than 100 participants, including foreign participants from Vietnam and Thailand, as well as the United States and countries in Europe. In the future, this symposium will be held once every 2 years, being hosted in turn by Japan, China, and Korea.

MatNavi has not only won a high evaluation as an extremely useful database from users in Japan and other countries, but is also recognized as one item that receives a high evaluation in external evaluations of the performance of NIMS as an organization. In April 2012, MatNavi received the NIMS President's Award for its operation and achievements to date, and also received the Minister's Prize from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) for Contribution to Promotion of Information Technology in the Information Technology Promotion Division.

Future issues

In the databases, new data are searched and used together with existing data as data continue to be updated. However, if data are not updated, they are no longer used and are deleted. In the past, the NIMS polymers database PoLyInfo extracted data from approximately 2000 literature sources, but due to budgetary restrictions, this is now a mere 600. Likewise, the data in the the inorganic materials database AtomWork was expanded and the number of accesses was rapidly increased 2 years ago, but because this was limited to data from more than 10 years ago, users have strongly requested further expansion. However, updating of this database is also difficult due to budgetary and contractual issues. Moreover, we have also had strong requests to expand the electronic structure computational database CompES.

As another problem, we do not have full-time expert personnel assigned to the MatNavi database project. We hope to improve this area in the future. Adoption of literature data for the polymers database has been done by a retired expert for many years, and although this ensures the reliability of the data, training of the next generation is urgently needed. Thus, further improvement is needed in various aspects.

We are striving to expand use of MatNavi in order to solve these issues. As one such effort, we have licensed NIMS Data Sheet online creep data and fatigue data to the Granta database, and we are also studying more effective use of our databases by domestic Japanese companies. As a future goal, we will endeavor to further expand our databases so as to contribute to research on new element strategies.

1) T. Ogata et al., Research and Development Supported by Materials Databases," Kinzoku, Vol. 81, No. 12 (2011), pp. 1005-1078.

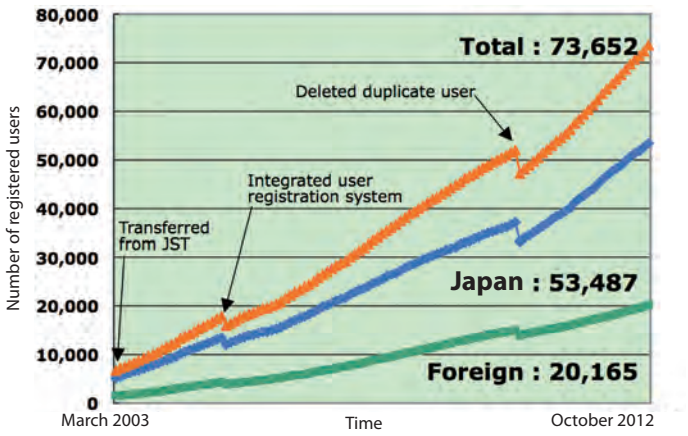


Fig. 3 Transition of number of registered users of MatNavi.

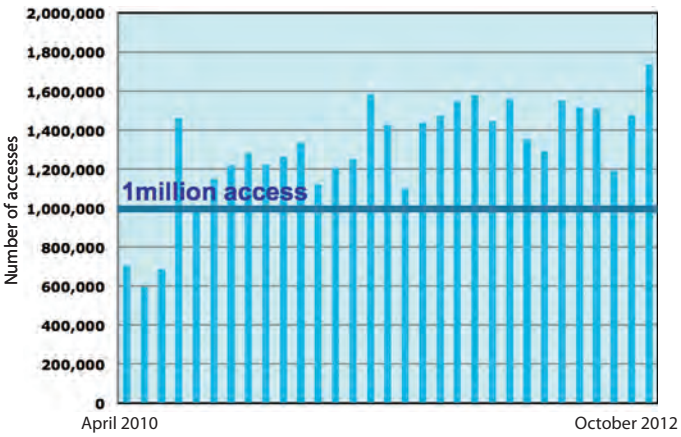


Fig. 4 Transition of access rate.

Toshio Ogata (Dr. Eng.) Completed the masters course at the University of Tokyo, Graduate School of Engineering, Department of Materials Engineering in 1979. From 1979, he was engaged in research, development, and property evaluation of cryogenic structural materials and international standardization at the National Research Institute for Metals (NRIM), and was later appointed Managing Director of the NIMS Materials Reliability Center. Since 2011, he has been Station Director of the NIMS Materials Information Station.

Inorganic Materials Database: AtomWork
Searching the True Nature of Materials from Materials Data

Materials Information Station,
Research Network and Facility Services Division
Yibin Xu

What is important for a materials database?

Materials databases do not simply provide data on the structures and properties of materials. They are essential for enabling the user to understand why a certain material has those properties. Databases are also important for providing users with design guidelines when designing materials with new properties. All these functions are aims of a materials database.

The properties of a material are determined by its composition and structure. Therefore, in a materials database, organic linkage of material property data and the material structure, composition, and component materials, and appropriate grouping of related materials are necessary. The NIMS Inorganic Materials Database "AtomWork" is one of the few databases in the world that provides all these functions.

The AtomWork data set

The predecessor of AtomWork was the materials database "PaulingFile," which was developed by the Japan Science and Technology Agency (JST). That database was developed cooperatively by the JST and the Swiss Material Phases Data System (MPDS) between 1995 and 2002, and included phase diagrams, crystal structures, and property data on inorganic materials drawn from the scientific literature. In 2008, the JST transferred the PaulingFile data set and data copyright to NIMS. Subsequently, NIMS carried out data supplementation and verification work in cooperation with MPDS. In the course of that work, powder X-ray diffraction patterns and 2D and 3D crystal structure images were calculated and prepared, and this was combined with the existing information to complete the AtomWork data set.

At present, AtomWork data comprise phase diagrams (15,000), crystal structures (82,000), X-ray powder diffraction (82,000), property data (55,000), and phase index data. X-ray powder diffraction data were simulated from crystal structure data using a program called RIETAN-FP. [1)] Four 2-dimensional images of the a-, b-, and c-axes and the diagonal direction were prepared for each crystal structure. Property data cover 100 types of properties, which are classified into 9 categories, such as mechanical, thermal and thermodynamic, optical, electronic, electrical properties, etc.

In AtomWork, the data reported in different literature items are treated as different materials. However, it is possible to group and compare related materials at each of the elemental, compound, and substance levels using phase index data. This phase index comprises the chemical system, chemical formula, and crystal structure. The chemical system identifies materials at the elemental level by comparing the constituent elements of materials. The chemical formula identifies the material at the compound level, and materials are identified at the substance level by a combination of the chemical formula and crystal structure.

Concrete search and data obtained

In the AtomWork material search screen (Fig. 1), in addition to the constituent elements or chemical formula of a material, the user can also designate the crystal structure. Search results are displayed at the elemental level, compound level, or substance level depending on this search condition.

For example, let us look at the results of a search by an Al-Ti chemical system (Fig. 2). Here, the results include 12 substances. If we look at the results of a search by the chemical formula Ti_3Al (Fig. 3), two substances are included. When the crystal structure hP8 was added to the chemical formula Ti_3Al (Fig. 4), it can be understood that one substance was designated as the search result. Furthermore, a list of all the literature in connection with materials containing the designated substance is also shown on the same screen. That list is classified into three categories, namely, crystal structure, X-ray diffraction, and properties, and can be displayed

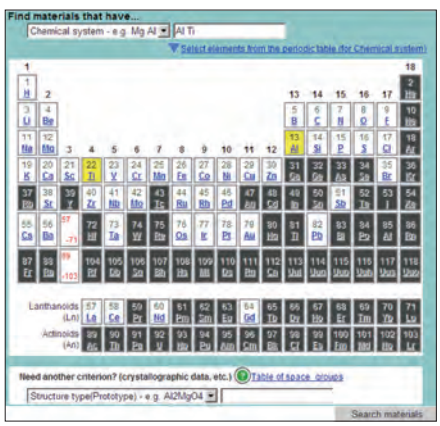


Fig. 1 Materials search screen.

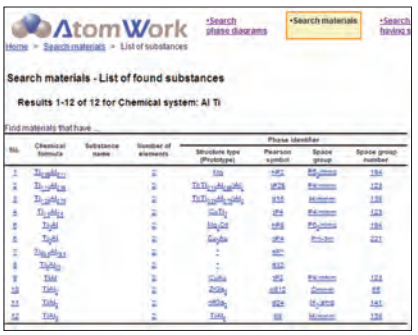


Fig. 2 Results of search by chemical system "Al-Ti."

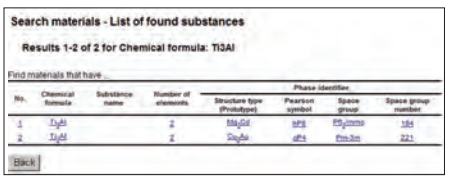


Fig. 3 Results of search by chemical formula "Ti_3Al."

Fig. 4 Results of search by chemical formula "Ti_3Al" + crystal structure "hP8."

by category. The content of the literature is displayed from that list (Fig. 5). In addition to the crystal lattice, atomic coordinates, etc., 2D and 3D images are also displayed. Data on crystal structures can be downloaded in the form of crystallographic information files (CIF) [2] that can be imported directly to many computational programs and crystal structure viewers.

In the same manner, property data can also be searched and displayed at the elemental level, compound level, substance level, and material level. For example, as can be understood from the results of a search by the condition "Existence of data on bulk modulus and chemical system Al-Ti " (Fig. 7), this search method is convenient for comparison of material properties with different chemical formulas or crystal structures, and for investigation of the effects of the chemical formula or crystal structure on the properties of materials.

When searching phase diagrams, if "Al" and "Ti" are input, a list of the phase diagrams of Al-Ti systems is displayed. The listed substances (i.e., phases) are tied to the search results of the respective substances.

Applications of AtomWork

The phase diagrams, crystal structures, and property data of substances are extremely important basic data for synthesis of materials, understanding of material properties, and design of new materials. By effectively using the functions of AtomWork not only to display the respective data, but also to group, and compare those data, it is possible to analyze the composition and structural elements of materials. Moreover, this can also be useful in prediction of material properties.

Furthermore, new data can be created by linkage of AtomWork with other computational science programs. For instance, it is possible to import crystal structure data to a first-principle calculation program and calculate electronic structures, and import property data for single phase materials to the composite material property prediction system [3] and calculate the properties of composite materials. A new database called the "NIMS Interfacial Thermal Conductance Database (ICT)," in which AtomWork data are actually used by these techniques, has also been opened in the NIMS MatNavi system. [4]

1) F. Izumi and K. Momma: Solid State Phenom. 130 (2007) 15.
2) International Union of Crystallography: CIF, http://www.iucr.org/resources/cif/.
3) NIMS Composite Materials Thermal Properties Prediction System CompoTherm,
4) NIMS Interfacial Thermal Conductance Database (ICT),

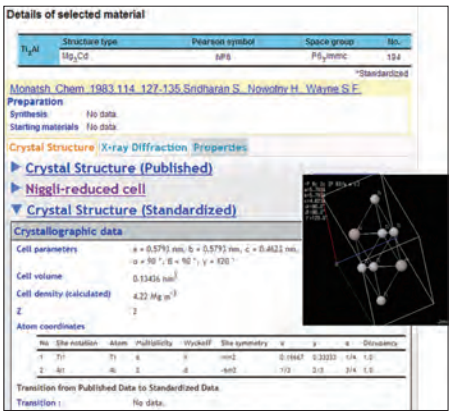


Fig. 5 Crystal structure display screen.

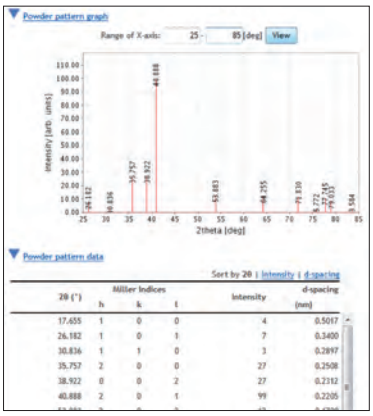


Fig. 6 X-ray powder diffraction display screen.

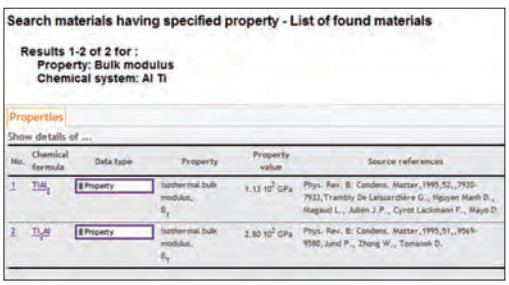


Fig. 7 Results of search by chemical system "Al-Ti" and property name "Bulk modulus."

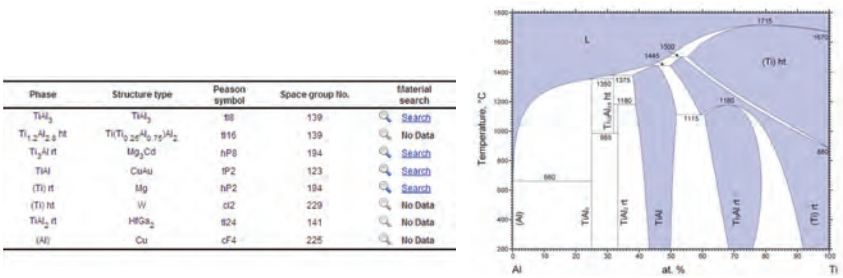


Fig. 8 Example of a phase diagram.

Yibin Xu Ph.D. (Engineering), Ph.D (Informatics) Completed the doctoral course with specialization in materials science at the School of Engineering, Shanghai Institute of Ceramics, Chinese Academy of Sciences in 1994, and received her Ph.D. in informatics from Nagoya University in 2007. Prior to her present position, she was a Postdoctoral Researcher at the National Industrial Research Institute of Nagoya and a member of the NIMS Database Station. She is currently a Principal Researcher in the NIMS Materials Information Station.

Polymers Database: PoLyInfo From its development to application

Materials Information Station, Research Network and Facility Services Division
Isao Kuwajima

Materials Information Station, Research Network and Facility Services Division
Junko Hosoya

Materials Information Station, Research Network and Facility Services Division
Yoshiko Shimizu

Materials Information Station, Research Network and Facility Services Division
Kentaro Mashita

Introduction

The Polymer Database PoLyInfo (http://polymer.nims.go.jp/en) is a database in which information necessary for material design using polymers is collected from the scientific literature and provided to registered users free of charge via the internet. This database contains information on polymer names, chemical structures, polymerization methods, processing methods, physical properties, measurement conditions, raw material monomers, etc. Property prediction system, nomenclature system and NMR database are also available as advanced functions.

Development of PoLyInfo

Development of PoLyInfo as one of the functional materials databases of the Japan Science and Technology Agency (JST) began in 1995, and a prototype was opened in 1998. In 2003, the database was transferred to NIMS. Over the past 10 years, NIMS has expanded its data and functions as one of the databases in the NIMS Materials Database MatNavi (http://mits.nims.go.jp/en).

Data sources and data collection

As data sources, PoLyInfo uses literature that clearly describes the chemical structure and provides measured values for physical properties from among the scientific literature containing information on polymers registered with the Chemical Abstracts Service (CAS). At present, data are collected from approximately 600 sources annually. The collected content includes chemical structures, features of materials, molecular weights, polymerization methods, processing methods, shape of test piece, crystal structures, physical properties, measurement conditions, raw material monomers, and other items. Data that can be collected are input in an original NIMS data format comprising approximately 1500 lines for one sample. A total of about 100 physical properties are included, centering on thermal properties, electrical properties, physiochemical properties, and mechanical properties, among others.

In PoLyInfo, NIMS also developed and operates an original chemical compound registry system for polymers called the "Polymer Dictionary" based on information collected from the scientific literature. The Dictionary summarizes the common parts of sample data, making it possible for users to search and identify substances based on the polymer name, chemical formula, and chemical structure. The work of collecting data from the literature and preparing the dictionary data is performed by retired polymer researchers from private companies, and is double-checked by an editor different from the person collecting the data. Including outside contractors, a total of 13 people are involved in the various aspects of PoLyInfo, ranging from data collection/editing and dictionary data preparation to actual system operation, etc. As of November 2012, available data covered 18,278 polymers, 1,537 polymer blends, 1,638 composites, 94,886 samples, 241,899 physical property points, 16,601 monomers and 13,721 selected literature items.

Search methods

The aims of PoLyInfo users include material development, product development, material selection, investigation of problems, and preparation of materials for teaching and lectures, reports, and scientific papers. We have prepared a variety of search functions to enable those users to obtain the information they require quickly.

In Polymer Search, the "Basic" function allows users to perform searches by inputting or selecting a name, class, chemical formula, material type, physical property, literature, etc. "Advanced" enables searches using more detailed conditions, in which users can designate copolymer or polymer blend component, additive/filler, average molecular weight, shape of test piece, degree of crystallinity, and up to 3 physical properties. Polymer Structure Search includes a "by Elements" function that allows users to designate the type and number of atomic groups contained in constitutional units, and a "by Modeling" function that makes it possible construct diagrams of constitutional units using a modeling tool and perform searches extending as far as their sequence and bonding relationships. "Easy Browse" functions include "Plotted data," which allows the user to draw graphs by selecting the object physical

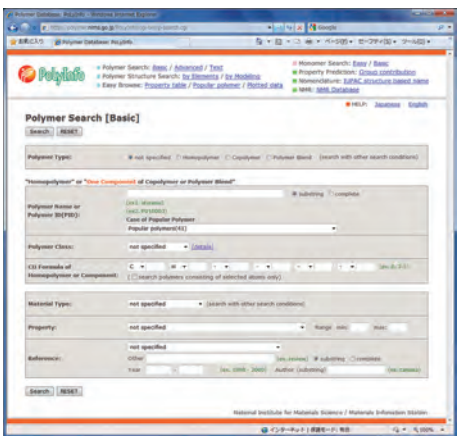


Fig. 1 "Basic" screen of Polymer Search.

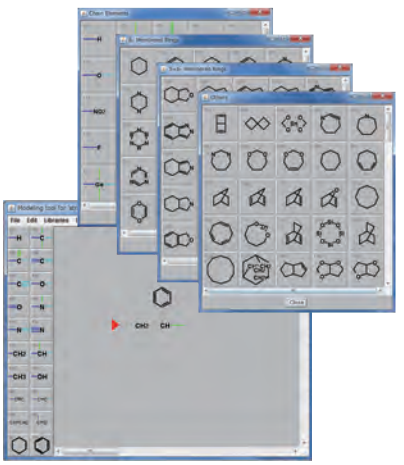


Fig. 2 "by Modeling" screen of Polymer Structure Search.

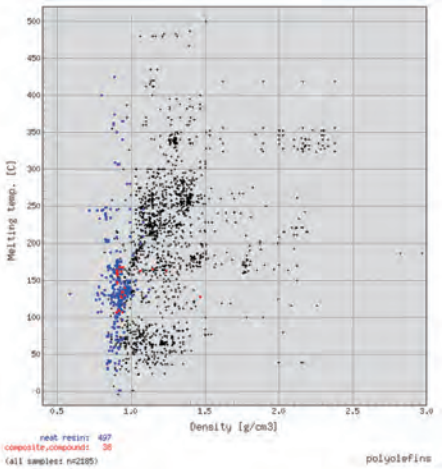


Fig. 3 "Plotted data" screen of Easy Browse (showing designation of the x-axis: density, y-axis: melting temperature, and class: polyolefins).

properties on the x- and y-axis and conduct searches from the range of the object physical values. It is also possible to perform searches from the monomers that are the raw materials for polymers, and in this case, the user can designate the monomer name, various registration numbers, classifications, molecular formulae, and molecular weights, and then jump to information on the polymers which are polymerized from the monomers that appear as "hits."

Advanced functions of PoLyInfo

The properties prediction system enables computation of the glass transition temperature, melting temperature, solubility parameter, surface tension, dielectric constant, refractive index, density, bulk modulus, shear modulus, tensile stress at break using the group contribution method. As predictive equations, the Van Krevelen equation is used, and the Van Krevelen parameter and PoLyInfo parameters optimized based on data collected in PoLyInfo are used as parameters. Predicted values can be compared with actual measured values collected in PoLyInfo. The nomenclature system enables automatic creation of structure based name conforming to IUPAC by diagraming constitutional units using the modeling tool. The NMR database provides ^{1}H and ^{13}C NMR spectral data and attribution data for 154 types of samples. Although links are possible from PoLyInfo polymer information, dedicated NMR functions which enable searches based on polymer conditions, polymer structures, and chemical shift are also provided.

Examples of use of PoLyInfo

Although various examples of use by users could be mentioned, the most common application is as standard reference data. Other applications include use as basic data for confirmation of general polymers, investigation when a polymer is unknown in the literature, and material design, as well as comparison with polymers prepared by the user, etc. Some users also employ PoLyInfo when developing new polymers in order to narrow the range of candidates and reduce the number of times that synthesis experiments must be performed by conducting PoLyInfo searches to determine the properties possessed by polymers with the object molecular structures. In research planning, PoLyInfo is used to propose similar materials, etc. when studying new products. In addition, some users use NMR information to identify the spectra of synthesized polymers, and some extract data from PoLyInfo as basic data for simulations. In the past, it was necessary to confirm information by obtaining books, scientific papers, and the like. This tedious, time-consuming process can now be performed instantly using the online database PoLyInfo.

Future issues

When PoLyInfo was originally developed, it was limited to only homopolymers, but the polymers handled have greatly expanded as a result of extension of the Polymer Dictionary in recent years. However, further improvement will be made in the future, as the system is still inadequate for multi-branched polymers. PoLyInfo users are not limited to specialists in polymers, as originally assumed, but include people from a wide range of industries and occupations that use polymers. In this connection, improvements in user-friendly search and display functions are necessary. Moreover, since it is difficult for any one institution to possess complete information, we plan to promote tie-ups with outside systems that are useful for users so as to provide a wider range of information. Finally, because the work of constructing and opening a materials database is not a one-time project, but rather, must be a long-term, on-going process, modeling of the organizational and budgetary aspects is the most important issue.

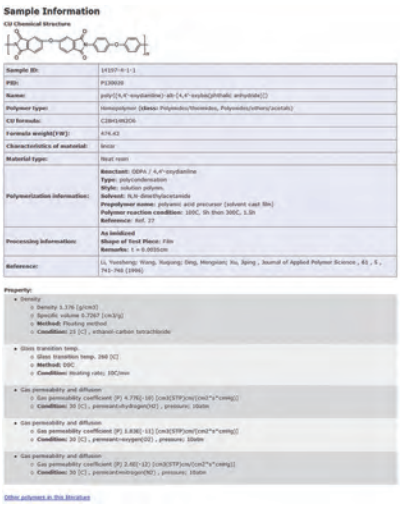


Fig. 4 "Sample Information" screen.

Fig. 5 Properties prediction result screen for PET (polyethylene terephtalate) using the group contribution method.

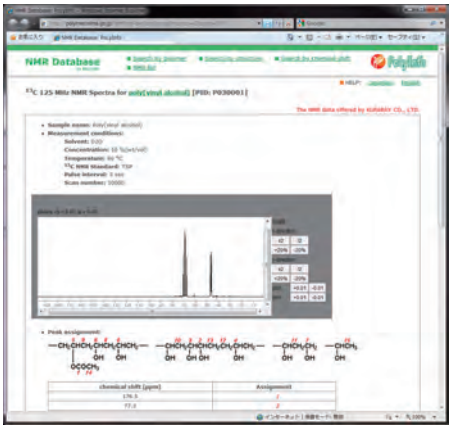


Fig. 6 NMR spectra screen showing ^{13}C 125MHz spectra of PVA (polyvinyl alcohol)).

Isao Kuwajima Completed the masters course at the Kogakuin University Graduate School of Engineering, Department of Industrial Chemistry in 2000. He has been a NIMS Researcher in the Materials Information Station in charge of development of PoLyInfo and MatNavi since 2002. **/ Junko Hosoya** Completed the Master's Program in Environmental Sciences at the University of Tsukuba Graduate School in 2000. Since joining Cosmo Sonic 21, she has been in charge of system development and operational control for MatNavi. **/ Yoshiko Shimizu** Graduated from Tamagawa University, Faculty of Agriculture, Department of Agricultural Chemistry in 1977. She is a research staff member of the NIMS Materials Information Station and has been in charge of PoLyInfo data management at JST and NIMS since 1997. **/ Kentaro Mashita** Ph.D. (Science) Graduated from the University of Tokyo, Faculty of Science, Department of Chemistry in 1967 and was then employed at Sumitomo Chemical Co., Ltd. He has been in charge of PoLyInfo data collection at JST and NIMS since 1999.

Metallic Materials Database: Kinzoku
Fatigue to Creep Rupture Properties — to the further evolution of database

Materials Information Station,
Research Network and Facility Services Division
Masayoshi Yamazaki

Materials Information Station,
Research Network and Facility Services Division
Junko Hosoya

A metallic materials database covering 500 types of materials and 3,500 heats

The NIMS Metallic Materials Database, Kinzoku (kinzoku means "metal" in Japanese) is the result of the reconstruction of various databases covering different researchers/research periods as single database in 2010. The database group consists of a database on pressure vessel materials, a database on nuclear materials, and the tensile properties, creep properties, creep rupture properties, and fatigue properties recorded in the NIMS structural materials data sheet online numerical databases. The database also contains extensive information on the basic properties of metallic materials, such as density, elastic modulus, Poisson's ratio, hardness, and toughness. Although strength data on iron and steel materials comprise a large part of the database, the database also includes information on aluminum alloys, titanium, and titanium alloys. In total, approximately 82,700 data items covering 500 types of materials and 3,500 heats (differences in manufacturing processes) are stored in this database.

The data in the NIMS structural materials data sheet are all for new materials that are not yet in use. However, the Kinzoku database also contains data on the toughness and creep rupture properties of aging Cr steel materials used in actual equipment such as pressure vessels, etc.

Continuing evolution of the Kinzoku database

As shown in Figure 1, Kinzoku enables users to select and search standard numbers (JIS, ASTM), material names (carbon steel, titanium, etc.), shape of the basic material (plate, bar, etc.), material history (new material, recycled material, aging material), chemical composition range, and various material properties on the screen.

Figure 2 shows an example of a search of the Poisson's ratio of low alloy steels. Although three numerical values are shown, it is possible to display the heat treatment conditions, etc. of the materials that show these respective values by jumping to the detail screen. Figure 3 shows the results of a search by the creep rupture properties of aging low alloy steel materials. Creep rupture curves for these data can be drawn either by heat or by a combination of multiple heats. Fig.4 shows the graph of the results of search in the giga cycle fatigue data.

Because creep, fatigue, and other properties of materials are affected by trace chemical components, the manufacturing process, heat treatment conditions, and other factors, there are differences in the strength properties of materials, even among materials specified by the same standard. Therefore, the detailed information screen of Kinzoku displays the chemical composition and heat treatment conditions together with the material property values.

In spite of these impressive features, the system of the Kinzoku Metallic Materials Database is considered to be still in the developmental stage. Further extension of both the materials and types of property values is planned in the future.

Fig. 1 Search screen of Kinzoku Metallic Materials Database.

Fig. 2 Example of results of a search of Poisson's ratio of low alloy steels.

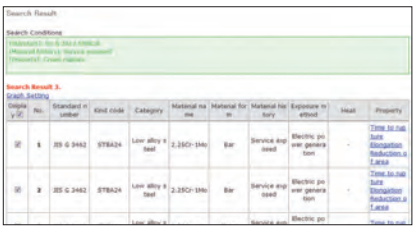


Fig. 3 Example of results of a search of creep rupture properties of aging low alloy steel materials.

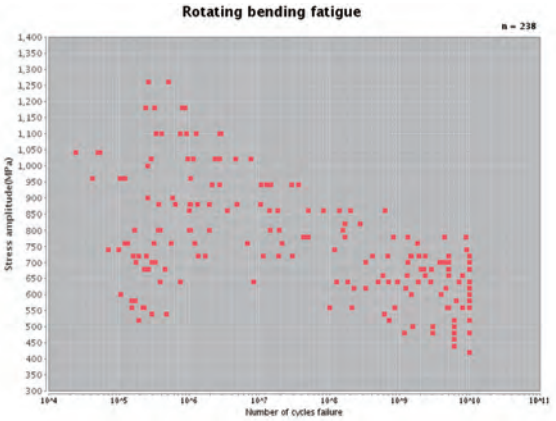


Fig. 4 Graph of the results of a search in the giga-cycle fatigue data.

Masayoshi Yamazaki Graduated from the Department of Mechanical Engineering, Shibaura Institute of Technology in 1972. Before appointment to his present position as NIMS Special Researcher, he was a member of the Creep Testing Department and the Mechanical Structure Research Department of the National Research Institute for Metals (NRIM) and the NIMS Database Station.
/ Junko Hosoya See profile on page 9.

From the User's Standpoint: The Traditions of Polymer Research and Future of Materials Development Linked by PoLyInfo

Separation Functional Materials Group,
Polymer Materials Unit, Advanced Key Technologies Division
Sadaki Samitsu

Polymer research to date

Polymers are widely used in various applications, from general-purpose materials like plastics and rubber to materials for optical communications, electronic devices, and medical applications, and have become one of the key groups of materials supporting society. NIMS is also actively engaged in leading-edge research on polymer materials with the aim of solving environmental and energy problems and contributing to the information and communication technology (see NIMS NOW, September 2012 edition).

Polymers were discovered about 100 years ago, and the first Nobel Prize for work in connection with polymers (macromolecular chemistry) was given to the German scientist Hermann Staudinger in 1953. Today, polymers with diverse molecular structures can be synthesized, and a wide range of material properties have been measured and evaluated. Japan is one of the world's leading countries in the polymer industry, and also holds a comparable position in the scientific world, having published a large number of outstanding research results in scientific papers worldwide.

On the other hand, together with the expansion in research, the number of published papers has also become enormous, and with each passing year, it is becoming more difficult to arrange the necessary data from published papers. This is not an easy matter even for experts who have been engaged in polymer research for many years, and may also become a serious bottleneck for students who are attempting to begin research on polymers, researchers in other fields, and engineers working in private companies.

A polymer database supporting research and development

The NIMS Polymer Database PoLyInfo demonstrates its effectiveness as a tool for overcoming these difficulties. PoLyInfo was constructed by comprehensively collecting and systematically organizing information in papers published throughout the world up to the present. It already covers as many as 100 types of physical properties such as thermal properties, mechanical properties, electrical properties, physiochemical properties, and others for polymer materials groups exceeding 20,000 types. Because a wide range of data from the literature is collected as digital data, PoLyInfo makes it possible to find the desired data at the desired time by using a personal computer information search function.

In my own research, I constantly use a diverse range of data, including mechanical properties such as modulus of elasticity, strength, etc., thermal properties such as melting point, glass transition temperature, and enthalpy of fusion, solution properties, and others. The most important advantage of PoLyInfo is that this system makes it possible for anyone to use this huge volume of property data on polymers in a simple manner. PoLyInfo is also promoting fusion between fields by enabling wide use of information that had been limited to specialists in polymers until now. Because this information is used throughout the world, not only by specialists, but also by materials researchers in the fields of metallic materials and inorganic materials, as well as researchers and company engineers in other fields such as chemistry, biotechnology, electronics, and machinery, PoLyInfo may contribute to the creation of hybrid materials with dramatically improved properties and the birth of new fields of application. From my own standpoint as one researcher engaged in polymer research, I wholeheartedly hope for the further development of the PoLyInfo system.

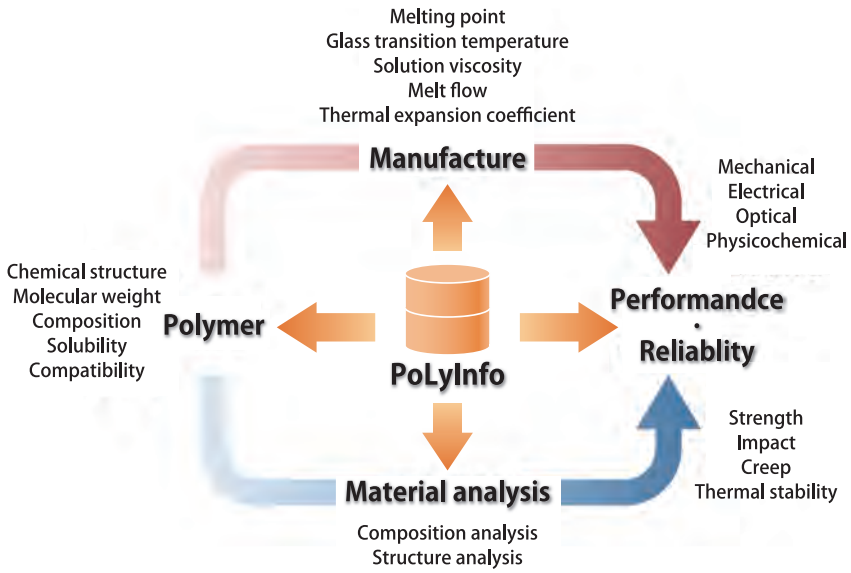


Fig. PoLyInfo provides strong support for scientific and industrial development of polymer materials.

Sadaki Samitsu Ph.D. (Engineering) Completed the doctoral course at the School of Engineering, University of Tokyo in 2006. Prior to appointment to his present position as NIMS Researcher in 2009, he was a Researcher at the Graduate School of Science, Kyoto University.

NIMS NEWS

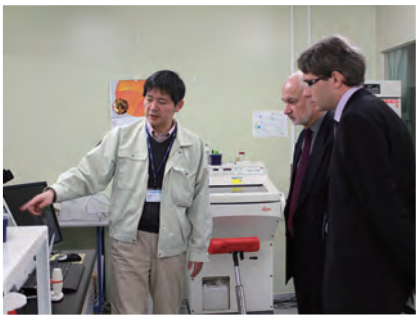
1 Slovak Republic Ambassador Visits NIMS

(Dec. 11, 2012) H.E. Mr. Drahomir STOS, Slovak Republic Ambassador Extraordinary and Plenipotentiary to Japan, accompanied by Mr. Branislav POCHABA, First Secretary, Department of Business and Economic of the embassy, paid a visit to NIMS President Prof. Ushioda.

The ambassador is working actively to promote research and personnel exchanges between Japan and Slovak and particularly interested in our effort for globalization and how to recruit and receive a researcher from overseas at NIMS.

During the meeting with President Ushioda, they exchanged opinion about the common issues including energy and rare-earth for the both countries poor in natural resources. They also discussed about future collaboration between NIMS and Slovakian academic society.

In addition to the meeting, they visited Nano-Integration Foundry and Bio-Organic Materials Facility at Nanotechnology Innovation Station.



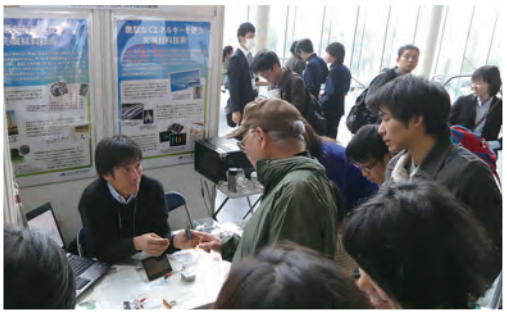
at Bio-Organic Materials Facility

2 NIMS Exhibits at Science Agora 2012

(Nov. 10-11, 2012) NIMS exhibited at "Science Agora 2012," which was held at the National Museum of Emerging Science and Innovation (Miraikan) under the sponsorship of the Japan Science and Technology Agency (JST), mainly for students and the general public. The motto of Science Agora is "A virtual, open place of assembly ("agora"), where science serves as a catalyst." Science Agora has been held each year since 2006, and is the largest science communication event in Japan.

At this year's Science Agora, NIMS exhibited for the first time as an institution. NIMS prepared a booth in the researcher zone, where representative NIMS research results were introduced, including phospors that were developed by NIMS and are now used in liquid crystal displays, ultra-high temperature alloys that NIMS developed to realize energy saving in jet engines, research protecting Japan's high performance magnets, and others. Recent research achievements at NIMS were also introduced in demonstrations by staff members.

A large number of visitors gathered at the NIMS booth during the two-day event, almost as though surrounding it, and there were large cheers when the presenters conducted demonstration experiments. In addition to children who were interested in the experiments, NIMS staff also received detailed questions on the content of research from adult visitors. Thus, this was a precious opportunity for achieving a wider knowledge of the most recent developments in materials research. During the two-day period, Science Agora attracted a total of 6,255 visitors.



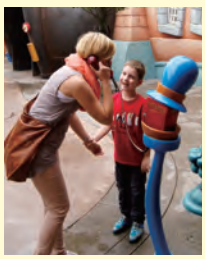
NIMS booth at Science Agora

Hello from NIMS

Dear NIMS NOW readers,

"Japan is one of the country I wanted to visit when I was younger. It is because Japan is unusual and mysterious country with fascinating culture and history. It is almost one year since I came to Japan and started to work with one of the best professionals I ever met. During this time I have acquired a lot of new skills and experience which is excellent for my future career. After a few months my family (wife and 6 year old son) joined me and our adventure has than began. We have attended a lot of cultural activities in order to get to know the people and the place around us. Of course, could not miss a visit to Tokyo's Disneyland which was a dream come true for our son. We spent our summer holiday on the ocean in the charming town of Shimoda. We were impressed by the beauty of nature around us, in particular by Shirahama Ohama Beach. Thanks to the hospitality of people who we have stayed with, we had the chance to taste Japanese cuisine. The sashimi served on a wooden boat made a great impression. There is no doubt we will miss Japan, and we really hope to return here someday. Maybe for a longer time…"

NIMS Summer Party



Tokyo Disney Resort

Tsukuba-san Shrine

Rafał Maksymilian Molak (Poland)
From December 2011 - present
Postdoctoral researcher
Coating Group, High Temp. Materials Unit, Environment and Energy Materials Division

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Public Relations Office, NIMS
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