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Inorganic Materials Database for Exploring the Nature of Material

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An inorganic materials database system, AtomWork, has been developed and released on the Internet. It includes the phase diagram, crystal structure, X-ray powder diffraction, and property data of more than 80,000 inorganic materials extracted from scientific literature. The feature of this database is that the information of the synthesis, identification, and property of materials is organically linked, which enables the data reported in different papers to be grouped and compared at four different levels: chemical system, compound, substance, and material. The database can provide users with a comprehensive overview of substances and necessary information to understand the relationships among chemical component, structure, and property.

1. Introduction

Understanding the relationships between the chemical component, structure, process, and property of materials is essential to material innovation. Phase diagram, crystal structure, and property data are important evidence showing how substances are formed from various chemical elements, how the atoms are structured, and what material properties are eventually produced; therefore, they are fundamental to the study of materials science and the development of new materials. These basic data are also indispensible as initial conditions used in many computational methods of materials science, such as first principles calculation, molecular dynamics simulation, and finite element method.

In the field of inorganic materials, the phase diagram, crystal structure, and property data have been published by many publishers, such as Springer,[1)] and ASM,[2,3)] etc. as handbooks since the 20th century. Now, most of these handbooks are also available in an electronic format as PDF files. However, the handbooks, even electronic handbooks, have a severe limitation in that the data published cannot be reorganized and exported into another form for use by other computational systems, for example, simulation and data mining systems.

Over the last 20 years, there has been a marked growth of materials databases. The primary advantage of a database system is that the preserved data can be optionally searched, retrieved, and exported into any defined format, so that information from different points of view can be obtained and further data processing by external computer systems is easy. The main database products currently available of inorganic materials are listed in Table I. Except for the Pauling File Binary Edition, all databases contain only one type of data, phase diagram or crystal structure, and therefore are not sufficient for the purpose of understanding the essential of materials, for which, as we mentioned above, comprehensive information of the chemical system, compound, structure, and property is required. The Pauling File Binary Edition is a database with linked phase diagram, crystal structure, and property information. Unfortunately, it contains only the data of binary systems; however, multinary systems are playing more and more important roles in present-day materials study and research. To meets the needs of today's materials study and innovation, this work has been carried out, aimed at the development of an inorganic materials database system that can provide fundamental data such as phase diagram, crystal structure, X-ray powder diffraction pattern and properties of binary and multinary inorganic chemical systems, substances, and materials. To reflect that "everything is made of atoms", the system is named AtomWork.

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2. AtomWork Data Content

From 1995 to 2002, Japan Science and Technology Agency (JST) carried out a collaborative project to collect the data of phase diagram, crystal structure, and properties of inorganic materials from scientific literature, together with Material Phases Data System (MPDS) in Switzerland. In 2008, JST transferred the copyright of the collected data to the National Institute for Materials Science (NIMS). Subsequently, NIMS spent two years completing and updating the data, in continuous cooperation with MPDS. Furthermore, based on the original data, computational data such as X-ray powder diffraction, and crystal structure image have been generated, and a new structured AtomWork inorganic materials data set has been created by NIMS. The content of AtomWork data is shown in Fig. 1. It can generally be divided into three parts: material data, phase index data, and literature data.

2.1 Material data

The materials data part includes the phase diagram, crystal structure, X-ray powder diffraction, and property data. The X-ray diffraction powder patterns were calculated from the crystal structure data using RIETAN-FP,[11)] a program developed by Izumi and Momma. Four crystal structure images along the directions of the *a*-, *b*-, and *c*-axes and the diagonal direction, were generated using the molecular visualization software Jmol.[12)] The property data includes nearly 100 properties classified into 9 categories: density, phase transitions, mechanical properties, thermal and thermodynamic properties, electronic and electrical properties, optical properties, ferroelectric properties, magnetic properties, and superconductor properties.

2.2 Phase index data

In AtomWork, the data extracted from different papers are treated as those for different materials. However, the data reported in a single paper is limited, so we often need to combine the data from different papers (materials) to obtain the information we require. For this purpose, criteria are

Table I. Main database products of inorganic materials.

Product	Data content	Publisher
ASM Alloy Phase Diagram Center[4)]	Phase diagram	ASM International (USA)
ACerS-NIST Phase Equilibria Diagrams Database[5)]	Phase diagram	American Ceramics Society, National Institute of Standards and Technology (USA)
ICSD Inorganic Crystal Structure Database[6)]	Crystal structure	FIZ Karlsruhe (Germany), National Institute of Standards and Technology (USA)
ICDD PDF-4[7)]	Crystal structure	International Centre for Diffraction Data (USA)
Pearson's Crystal Data[8)]	Crystal structure	ASM International (USA)
CRYSTMET[9)]	Crystal structure	Toth Information Systems, Inc. (Canada)
Pauling File Binary Edition[10)]	Phase diagram, crystal structure, property of binary system	ASM International (USA)

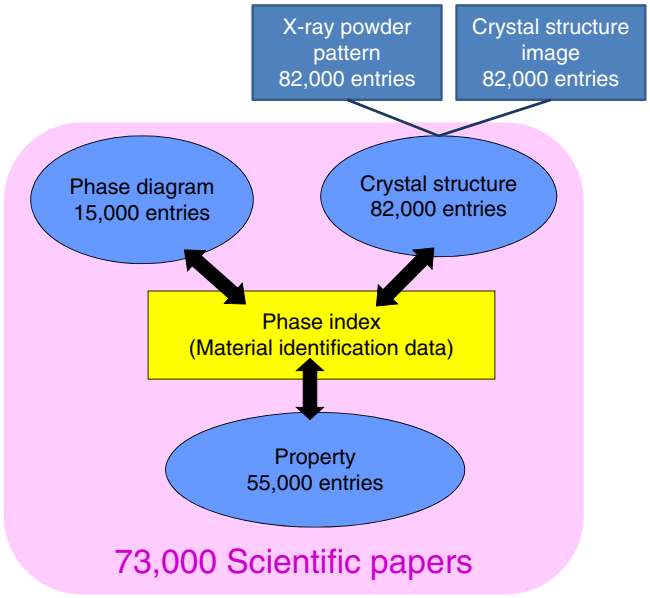

Fig. 1. (Color online) Data content of AtomWork data set.

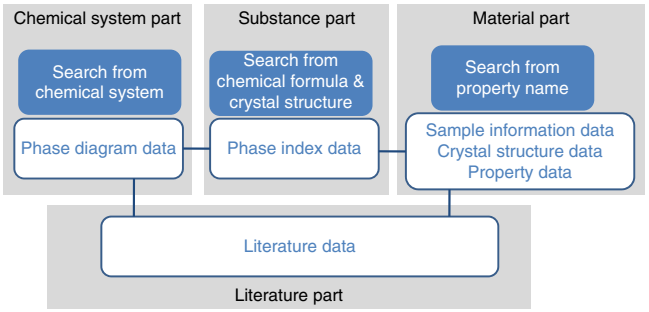

Fig. 2. (Color online) Architecture of AtomWork database system.

needed to judge whether and how these materials are related. Phase index is such a data set.

The phase index data includes chemical system, chemical formula, and crystal structure. The chemical system is used to identify a material at the level of element, chemical formula at the level of compound, and chemical formula together with crystal structure identifies a material at the level of substance. With the phase index data, materials can be grouped according to their intrinsic relations at different levels. Materials with the same chemical formula and crystal structure belong to the same substance, so that the material data can usually be combined and compared. For materials belonging to different substances, they may be linked and compared at the level of either chemical element or compound.

To represent the crystal structure, structure type (prototype), Pearson symbol, and space group name/number are used, since each of these representation systems has its own criteria for classifying the crystal structures. For example, the phase index of sapphire is Al_2O_3 (chemical formula), Al_2O_3 (structure type), hR30 (Pearson symbol), $R\bar{3}c$ (space group name), and 167 (space group number).

2.3 Literature data

The literature data includes the publication information, such as the paper title, journal, and author of the source literature. A digital object identifier (DOI)[13)] is available for about half of the documents, whereby users can access the web sources of the documents directly.

3. Database System

The database system provides the functions of search, retrieval and display of the data content. Depending on the operation logic of the database system, a data set can be viewed from different angles and therefore used for different purposes. For example, with the same data set of crystal structure, the PDF-4 database system is developed mainly for the identification of a substance from the X-ray powder diffraction pattern; meanwhile, Pearson's Crystal Data is for the user to look up the crystal structure of a known substance.

The purpose of AtomWork is to provide users a comprehensive view from atom to material; thus, an original database system structure and logic are needed. The greatest difference of AtomWork from the other existing inorganic materials databases is that it covers multilayer information from chemical system to substance and to material. Thus, the main architecture of AtomWork, as shown in Fig. 2, includes four parts: (1) the chemical system part, which provides the functions of management, search, and display of phase diagrams; (2) the substance part, which manages the phase index data and the links between the phase index and the material data. It also provides the function of search for a material from the chemical formula and the crystal

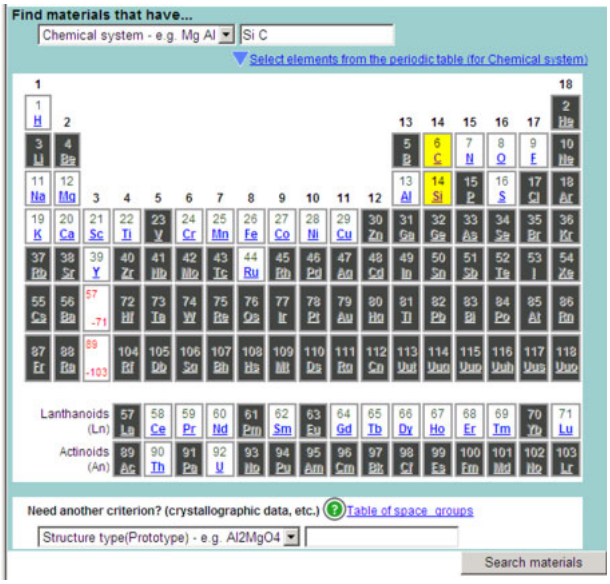

Fig. 3. (Color online) Interfaces of search material by selecting elements on the periodic table.

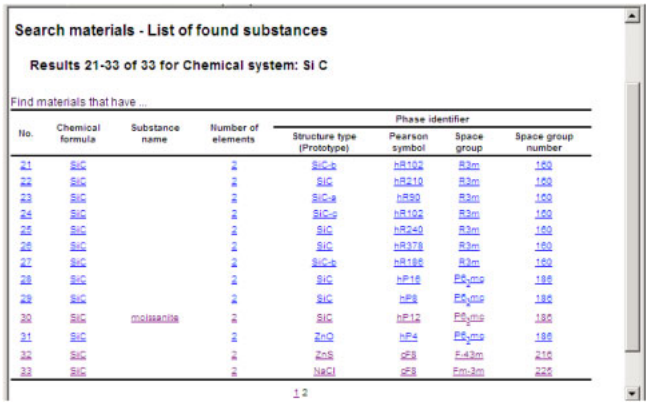

Fig. 4. (Color online) Search result of substances made of Si and C. More than 30 substances have been found for SiC.

Fig. 5. (Color online) List of papers for SiC with crystal structure of ZnS/cF8/$F\bar{4}3m$. By combining the information reported in different papers, a comprehensive image of the crystal structure and property of this substance is available.

structure; (3) the material part, which manages the data of sample information and the crystal structure and property data measured on the samples. The search function for materials from the property name is executed by this part; (4) the literature part, which contains bibliographic data of the original papers.

AtomWork is a web-based system developed with Java language and run on a Linux server. To use the system, a user needs only a web browser. Three search interfaces are available: search phase diagrams, search materials, and search materials having a specified property.

4. Explore the Nature of a Material Using Database

In this section, we will show how to obtain comprehensive knowledge of a substance by combining data reported by different researchers, and explore the relationships between chemical component, structure, and property using AtomWork, by taking SiC as a case study.

4.1 Substances made of Si and C

By selecting Si and C on the periodic table of the search materials interface shown in Fig. 3, we can get a list of the substances made of Si and C elements. The total list includes 33 substances and a part of them is shown in Fig. 4. From this result, we know that three compounds, $Si_{0.875}C_{1.25}$, $Si_{1.25}C_{0.875}$, and SiC (the first two are not shown in Fig. 4), can be formed by Si and C. Different compounds have different crystal structures. Furthermore, the SiC compound has more than 30 types of crystal structure, i.e., more than 30 different substances can be constructed by different spatial architectures of the SiC molecules.

Figure 5 shows a list of the papers containing the data of SiC with the crystal structure of ZnS/cF8/$F\bar{4}3m$. A total of 37 papers is found. Each paper is introduced by an icon indicating the data type, crystal structure/X-ray diffraction, or property. Data is displayed for every paper, since the samples in different papers are considered different materials. A summary of the description in each paper to identify the material, such as synthesis condition, and microstructure, is displayed if available, in addition to the common substance information.

4.2 Display of crystal structure

The crystal structure data extracted from the paper with the icon of "crystal structure/X-ray diffraction" in Fig. 5 is displayed in Fig. 6. The crystallographic data include the published data, standardized data, and Niggli-reduced cell data. If available, the synthesis and process of the sample may also be displayed on the same page.

The crystal structures can be viewed as both two- and three-dimensional graphs. For each crystal structure, four two-dimensional pictures of crystal structure, along the directions of the *a*-, *b*-, and *c*-axes and the diagonal direction, are available. Three-dimensional graphs are displayed interactively by a Java applet Jmol.[12] The three-dimensional crystal structure graph of SiC ZnS/cF8/$F\bar{4}3m$ is shown in Fig. 6.

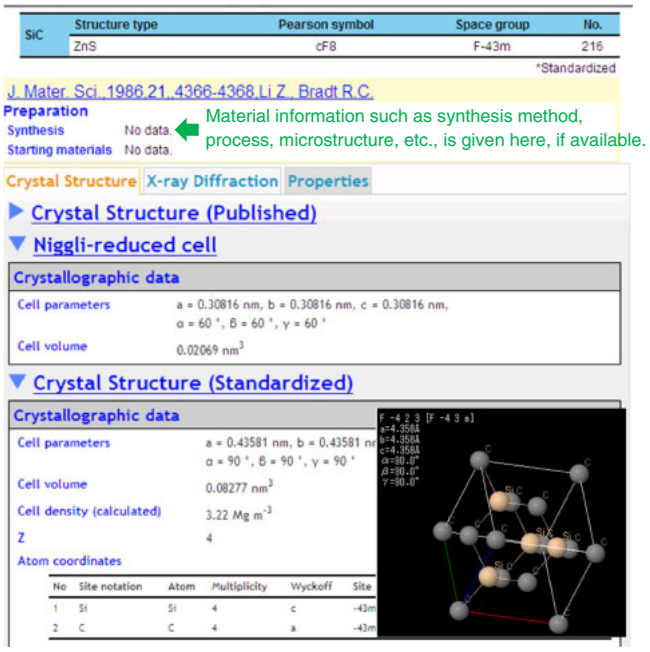

Fig. 6. (Color online) Crystal structure of SiC ZnS/cF8/$F\bar{4}3m$.

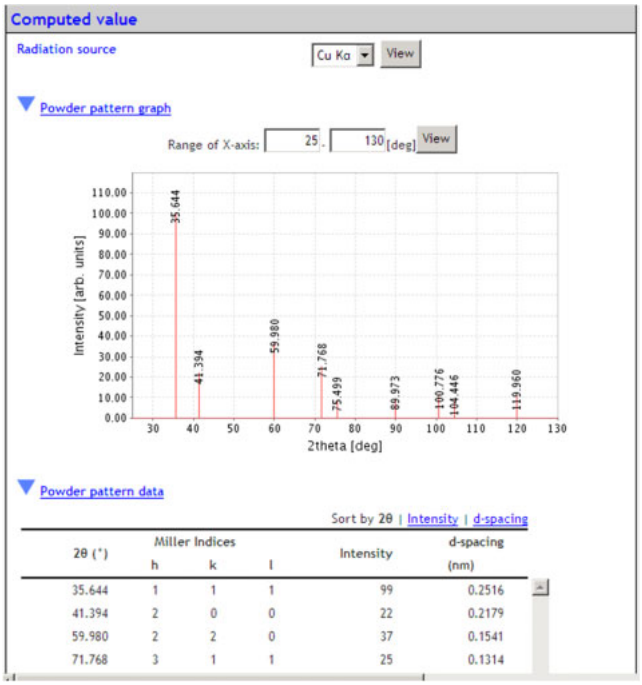

Fig. 7. (Color online) X-ray diffraction powder pattern of SiC ZnS/cF8/$F\bar{4}3m$.

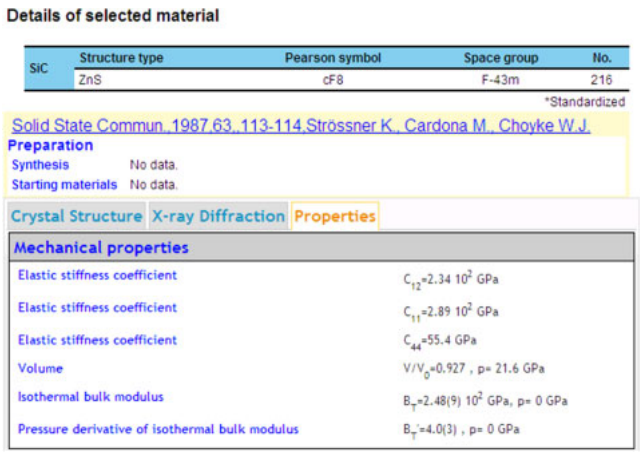

Fig. 8. (Color online) Mechanical property of SiC ZnS/cF8/$F\bar{4}3m$.

The crystal structures can also be exported as a crystallographic information file (CIF),[14] a file format that can be read by almost all crystal structure analysis software, so that they can be easily used by other computational and simulation software.

4.3 Display of X-ray diffraction pattern

X-ray diffraction is one of the most commonly used methods of identifying a substance. The plot and data table of the X-ray diffraction powder pattern of SiC ZnS/cF8/$F\bar{4}3m$ calculated from the crystal structure data is also available in AtomWork, as shown in Fig. 7.

4.4 Display of material property

The property data of SiC ZnS/cF8/$F\bar{4}3m$ extracted from one of the above papers is shown in Fig. 8. Similarly, other properties of the same substance can be obtained from other papers listed in Fig. 5. Although each paper focuses on a specific aspect of the substance, a comprehensive image including the crystal structure and various properties can be obtained by combining the information from different papers.

Material properties can also be searched using the property search function by specifying the property name. Figure 9 shows the search results for "energy gap" (band gap) and chemical formula "SiC". Different band gaps have been reported. However, by clicking on the hyperlink of each item, we can find that, in fact, these band gap data were measured on different SiC substances, i.e., materials with different crystal structures. On the basis of this information, we can analyze the dependence of the band gap on the crystal structure. On the other hand, if two materials that belong to the same substance show different properties, the difference is most likely caused by the features of the material, such as microstructure, surface, and interface.

4.5 Display of phase diagram

Phase diagrams provide information on compound formation and phase transition, which is important for the synthesis of a material. One of the phase diagrams of the Si–C system in AtomWork is shown in Fig. 10. We can see that the phase SiC 3C is formed at an atomic percentage of 50% for both C and Si at a temperature below 2000 °C. The phase transforms to SiC 2H when the temperature rises to above 2000 °C. The phase index data corresponding to each phase, bibliographic data of the source document, and a brief description of the experiment are also displayed. By clicking on the hyperlink of the phase index data, one can go directly to the crystal structure and property page of the substance.

5. Conclusions

During the long history of materials development and analysis, a large amount of data has been accumulated. How to preserve and make the best use of this intelligent wealth is an important subject to today's material researchers. In

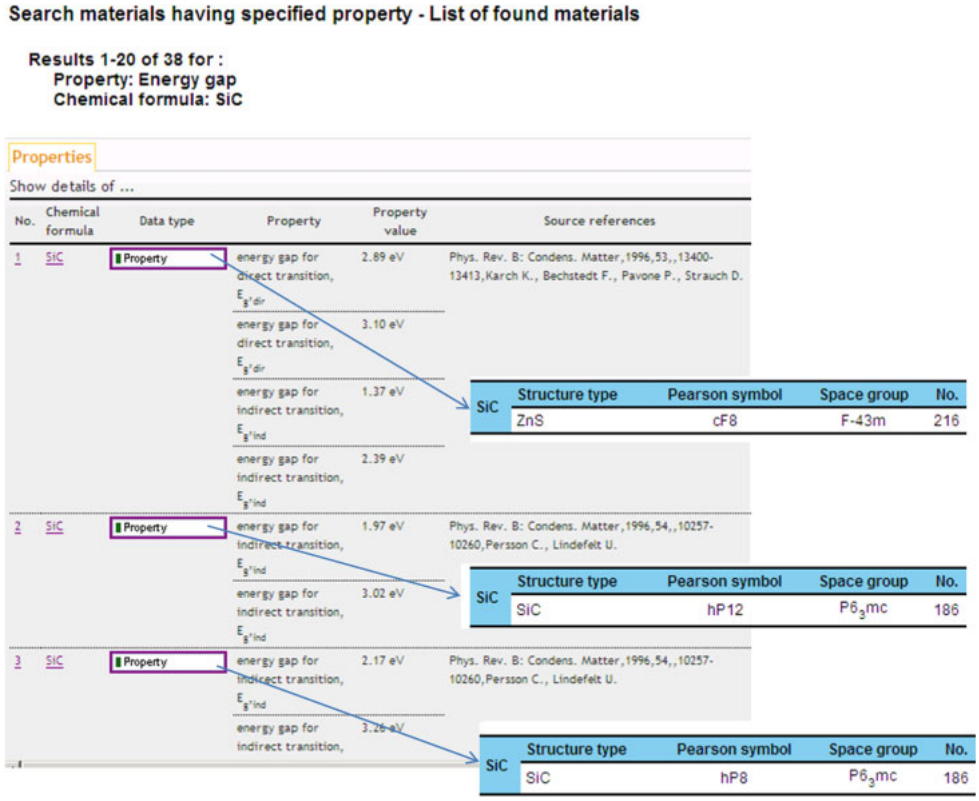

Fig. 9. (Color online) Search result of the band gap of SiC. Properties of materials with different crystal structures can be compared.

Phase	Structure type	Peason symbol	Space group No.	Material search
(Si)	C	cF8	227	Search
SiC 3C	ZnS	cF8	216	Search
SiC 2H	ZnO	hP4	186	Search
(C) gra	C-a	hP4	194	No Data

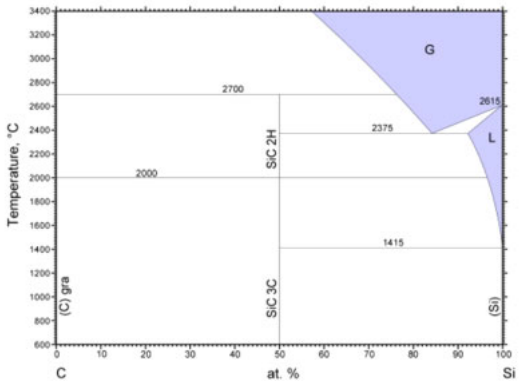

Fig. 10. (Color online) Phase diagram of Si–C system, which shows the condition of compound formation and phase transition of SiC.

this paper, we reported our work on the development of an inorganic materials database, AtomWork, which has been launched on the Web site of NIMS Materials Databases.[15,16] In this system, the synthesis condition, crystal structure, X-ray identification, and properties of substances are organically linked to each other. It provides users a comprehensive image of a substance, as well as the necessary information to analyze the relationships between the chemical component, structure, and property. We expect that this system will be of help to researchers and engineers in this field in understanding the essentials of materials science and to explore new ideas of material design and development.

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